High order Runge-Kutta-Nyström splitting methods for the Vlasov-Poisson equation

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Abstract

In this work, we derive the order conditions for fourth order time splitting schemes in the case of the $1D$ Vlasov-Poisson system. Computations to obtain such conditions are motivated by the specific Poisson structure of the Vlasov-Poisson system : this structure is similar to Runge-Kutta-Nyström systems. The obtained conditions are proved to be the same as RKN conditions derived for ODE up to the fourth order. Numerical results are performed and show the benefit of using high order splitting schemes in that context.

1 Introduction

Frequently, the Vlasov equation is solved numerically with particles methods. Even if they can reproduce realistic physical phenomena, they are well known to be noisy and slowly convergent when more particles are considered in the simulation. To remedy this, the so-called Eulerian method (which uses a grid of the phase space) has known an important expansion these last decades. Indeed, due to the increase of the machines performance, the simulation of charged particles by using Vlasov equation can be performed in realistic configurations. However, these simulations are still computationally very expensive in high dimensions and a lot has to be done at a more theoritical level to make simulations faster. For example, the use of high order methods is classical when one speaks about space or velocity discretization. However, for the simulation of Vlasov-Poisson systems, the use of high order methods in time is not well developed; generally, only the classical Strang splitting is used and analyzed; see however pioneering works of [15, 10] following [16] or the recent work of [13] in the linear case. We mention also the work [9], which tells us that that the increase of order of discretization in space should be followed with an increase of order in time.

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On the other side, a literature exists around the construction of high order methods for ODE (see [3, 2, 8, 14]). The main goal of this work is to construct high order splitting schemes for the nonlinear Vlasov-Poisson PDE system by the light of these recent references.

We consider here the $1D$ Vlasov-Poisson system satisfied by the distribution function $f(t,x,v)$ which depends on the time $t \geq 0$, the spatial direction $x \in [0,L]$ and the velocity $v \in \mathbb{R}$. We assume that the smooth initial data $f_0(x,v) := f(0,x,v)$ is compactly supported in v, L-periodic in x, and satisfies the relation

$$\frac{1}{L}\int_{\mathbb{R}}\int_0^L f_0(x,v)\mathrm{d}x\mathrm{d}v = 1. \tag{1.1}$$

The Vlasov-Poisson equation is then written

$$\partial_t f + v\partial_x f + E[f]\partial_v f = 0, \tag{1.2}$$

where the electric field is given from the solution f through the formula

$$E[f](x) = \partial_x^{-1}\left[\int_{\mathbb{R}} f(x,v)\mathrm{d}v - 1\right] = \int_0^L K(x,y)\left(\int_{\mathbb{R}} f(y,w)\mathrm{d}w - 1\right)\mathrm{d}y, \tag{1.3}$$

where

$$K(x,y) = \frac{y}{L}, \text{ if } 0 \leq y \leq x, \;\; K(x,y) = \frac{y}{L} - 1, \text{ if } x \leq y \leq L,$$

that is ∂_x^{-1} is the inverse of the derivative operator acting on L-periodic functions with zero average.

The equation (1.2) is endowed with a Poisson structure that we describe precisely in Section 2. The corresponding Hamiltonian energy is given by the functional

$$\begin{aligned} H[f] &= \frac{1}{2L}\int_0^L\int_{\mathbb{R}} v^2 f(x,v)\mathrm{d}x\mathrm{d}v + \frac{1}{2L}\int_0^L \big(E[f](x)\big)^2\mathrm{d}x \\ &=: T[f] + U[f] \end{aligned} \tag{1.4}$$

which is preserved along the solution of (1.2). The presence of Casimirs in the Poisson structure ensures the following preservation laws for all times $t > 0$ and all $k \in \mathbb{N}$:

$$\frac{1}{L}\int_0^L\int_{\mathbb{R}} f(t,x,v)^k\mathrm{d}x\mathrm{d}v = \frac{1}{L}\int_0^L\int_{\mathbb{R}} f_0(x,v)^k\mathrm{d}x\mathrm{d}v. \tag{1.5}$$

Note that for $k = 1$ this ensures - with the help of (1.1) - the well-posedness of (1.3) for all times.

The splitting methods we consider in this work are based on the decomposition $H = T + U$ of the Hamiltonian (1.4). As we will see below the Hamiltonian equations associated with T and U are simply the equations

$$\partial_t f + v\partial_x f = 0 \quad \text{and} \quad \partial_t f + E[f]\partial_v f = 0 \tag{1.6}$$

respectively. Both these equations can be solved explicitely using the characteristics formula. For a given initial condition f_0, the solution of the first one is given by $f(t,x,v) = f_0(x - tv, v)$ and the second by the relation $f(t,x,v) = f_0(x, v - tE[f_0])$ after noticing that $E[f_0]$ is a constant of motion in the evolution of the Hamiltonian system associated with U.

Hence we are naturally led to study the following class of methods: For a given $s \in \mathbb{N}^*$, coefficients a_p, $p = 0, \ldots, 2s$, and a time step $\Delta t > 0$, we define the splitting scheme with $2s+1$ stages by the relations $g_1(x,v) = f_0(x - a_0 \Delta t v, v)$, and

$$\begin{aligned} g_{2j}(x,v) &= g_{2j-1}(x, v - a_{2j-1} E[g_{2j-1}](x)\Delta t), \\ g_{2j+1}(x,v) &= g_{2j}(x - a_{2j}\, v\, \Delta t, v), \end{aligned} \tag{1.7}$$

for $j = 1, \ldots, 2s$. The quantity $g_{2s+1}(x,v)$ should be an approximation of $f(\Delta t, x, v)$.

As composition of exact flows of Hamiltonians T and U, such schemes are (infinite dimensional) Poisson integrators in the sense of [8, Chapter VII]. In particular they preserve the Casimirs for all times. Note that in this work, we do not address the delicate question of space approximation and focus on time discretization effects (see [1, 4, 11]).

As long as the finite dimensional case is concerned, many works exist concerning the analysis of order conditions for splitting methods (see in particular [3, 8, 2] and the references therein). In this setting, let us recall that for ordinary differential systems of the form

$$\dot{y}(t) = f_A(y(t)) + f_B(y(t)), \quad y(0) = y_0 \in \mathbb{R}^n, \tag{1.8}$$

with $f_A, f_B : \mathbb{R}^n \to \mathbb{R}^n$, then denoting by $\mathcal{L}_A$ and $\mathcal{L}_B$ the Lie operators associated with these vector fields, a splitting method of order d is a composition of the form

$$\prod_{i=1}^{2s+1} \exp(c_i \Delta t \mathcal{L}_A) \exp(d_i \Delta t \mathcal{L}_B) = \exp(\Delta t \mathcal{L}_{A+B}) + O((\Delta t)^{d+1}),$$

with appropriate coefficients c_i, d_i. Here, $\exp(t\mathcal{L}_{A+B})$ is meant as the exact flow of the ODE system (1.8) associated with the vector field $f_A + f_B$.

In the particular case where f_A and f_B satisfy the relation

$$[[[\mathcal{L}_A, \mathcal{L}_B], \mathcal{L}_B], \mathcal{L}_B] = 0, \tag{1.9}$$

where $[\cdot\,,\cdot]$ denotes the Lie bracket of two operators, then the algebraic order conditions on the coefficients c_i and d_i can be simplified to a large extent, and we speak about Runge Kutta Nyström (RKN) methods (see [2] for a review). A particular case of importance concerns second order systems of the form $\ddot{y}(t) = -\nabla P(y(t))$ for which the condition (1.9) can be easily recast in terms of (finite dimensional) Poisson bracket between the kinetic and potential energies.

Concerning now the Vlasov-Poisson case, we will see in Section 2 that the functionals T and U in the decomposition (1.4) satisfy the following formal RKN type relation

$$\{\{\{T, U\}_f, U\}_f, U\}_f = 0, \tag{1.10}$$

where $\{\cdot,\cdot\}_f$ is the Poisson bracket associated with the infinite dimensional Poisson structure. In fact the Vlasov-Poisson system even satisfies the stronger property

$$\{\{T,U\}_f,U\}_f = 2U.$$

This means that we can hope to have even simpler algebraic order conditions as those of RKN type for the specific Vlasov-Poisson system. However, as we will see below, this has no impact on the conditions up to the order 4 included.

To tackle the difficulties inherent to the infinite dimensional nature of the equation, we choose to work at the level of the characteristics representation of (1.2): Let us recall that if $(X(t;h,x,v),V(t;h,x,v))$ denotes the solution of the characteristics at time t whose values at time h were (x,v), we have

$$X(t;h,x,v) = x + \int_h^t V(\sigma;h,x,v)d\sigma, \tag{1.11}$$

$$V(t;h,x,v) = v + \int_h^t E(\sigma,X(\sigma;h,x,v))d\sigma, \tag{1.12}$$

with the electric field

$$E(t,x) = \int_0^L K(x,y)\left(\int_{\mathbb{R}} f_0(X(0;t,y,w),V(0;t,y,w))\mathrm{d}w - 1\right)\mathrm{d}y, \tag{1.13}$$

where f_0 is the initial condition. The solution of the Vlasov-Poisson equation is given by

$$f(t,x,v) = f_0(X(0;t,x,v),V(0;t,x,v)).$$

Now associated with the splitting scheme (1.7) we define the forward numerical characteristics through the relation

$$g_{2s+1}(X_s(\Delta t;0,x,v),V_s(\Delta t;0,x,v)) = f(\Delta t,X(\Delta t;0,x,v),V(\Delta t;0,x,v)). \tag{1.14}$$

The strategy we use is then to derive the conditions satisfied by the coefficients a_j, $j = 0,\dots,2s$, so that the forward numerical characteristics are fourth order approximations of the (continuous) characteristics, that is

$$X_s(\Delta t;0,x,v) = X(\Delta t;0,x,v) + O(\Delta t^5),\ \ V_s(\Delta t;0,x,v) = V(\Delta t;0,x,v) + O(\Delta t^5).$$

We assume here enough regularity on the initial data f_0 so that the computation of the time derivatives can be done. Using this characteristics representation, we can directly derive the algebraic order conditions without manipulating the delicate infinite dimensional Lie operators associated with T and U and acting on Banach spaces. By elementary computations, we are thus able to prove that the order conditions are the same than RKN methods, for the order ≤ 4. This strategy could also be applied to develop and analyse other schemes following [12],[13].

Concerning the literature, a fourth order splitting scheme (the so called triple jump scheme) has already been used for Vlasov simulations in [15, 10], following [16]. In [15], even higher order schemes (Yoshida type schemes [16] which are of arbitrarily

even order) have been tested, and the conservation of the total energy has been shown (numerically) to be of order $O(\Delta t^d)$, with d the order of the scheme. See also the recent work [12] where another similar scheme has been developed. A fourth order scheme has also been introduced recently and analyzed in [13] for the linearized Vlasov equation. To our knowledge a systematic analysis of fourth order splitting schemes of the form (1.7) has never been tackled for the Vlasov-Poisson system.
In Section 2, we introduce the Poisson structure and prove the RKN characterization, which is formally valid for schemes of arbitrary order. Section 3 is intended to the statement of the results for the elementary computations in the case of the order ≤ 4. Numerical results are shown in Section 4. For this, instead of using only Yoshida type schemes, we use some optimized coefficients developed in [3]. We observe that the energy conservation is improved even better. Finally, in Section 5, proofs of the results of Section 3 are given.

2 Poisson structure

In this section, we study the Poisson structure of the Vlasov-Poisson equation. This enables to make the link between the Hamiltonian structure at the ordinary differential equation level. Indeed, using the Poisson structure formalism, the Vlasov-Poisson equation can be written in terms of a Hamiltonian functional associated to the Poisson bracket $\{\cdot,\cdot\}_f$. In all the sequel, we will assume that the functions considered are smooth enough so that all the calculations make sense.

2.1 Generalities on the Vlasov-Poisson system

Let us recall that the phase space $(x, v) \in [0, L] \times \mathbb{R}$ is equipped with the standard Hamiltonian structure associated with the (finite dimensional) Poisson bracket $\{f, g\} = \partial_x f \partial_v g - \partial_v f \partial_x g$ where f and g are two smooth functions of (x, v). With this notation, we can rewrite the Vlasov-Poisson equation as

$$\dot{f} - \{h[f], f\} = 0,$$

where the dot means the time derivative, and where

$$h[f](x, v) = \frac{v^2}{2} + \phi[f](x),$$

with

$$\phi(f; x) = -\partial_{xx}^{-1}\left[\int_{\mathbb{R}} f(x, v)\mathrm{d}v - 1\right] = -\partial_x^{-1} E[f](x).$$

Considering the two functionals $T[f]$ and $U[f]$ defined in (1.4) we can calculate explicitely their Frechet derivatives which are given by

$$\frac{\delta T}{\delta f}[f] = \frac{v^2}{2} \quad \text{and} \quad \frac{\delta U}{\delta f}[f] = \phi[f](x).$$

Owing to the relation $H = T + U$, the Vlasov-Poisson equation can be written

$$\dot{f} - \{\frac{\delta H}{\delta f}[f], f\} = 0. \tag{2.1}$$

The previous equation is a Hamiltonian equation for the Poisson structure associated with the following Poisson bracket: For two functionals $H[f]$ and $G[f]$, we set

$$\{H, G\}_f = \frac{1}{L}\int_0^L \int_{\mathbb{R}} \frac{\delta H}{\delta f}\{\frac{\delta G}{\delta f}, f\}\mathrm{d}x\mathrm{d}v = -\{G, H\}_f, \tag{2.2}$$

where the Fréchet functionals are evaluated in f. Note the the skew-symmetry is obtained using the relation

$$\{fg, h\} = f\{g, h\} + g\{f, h\},$$

for three functions of (x, v) and the fact that the integral in (x, v) of a Poisson bracket of two functions always vanishes. Let $\varphi : \mathbb{R} \to \mathbb{R}$ be a smooth function, and consider the functional

$$\Phi[f] := \frac{1}{L}\int_0^L \int_{\mathbb{R}} \varphi(f(x, v))\mathrm{d}x\mathrm{d}v. \tag{2.3}$$

Its Fréchet derivative is $\frac{\delta \Phi[f]}{\delta f} = \varphi'(f)$ and using the definition (2.2), we can observe that for *all* Hamiltonian functional H, we have

$$\{H, \Phi\} = \frac{1}{L}\int_0^L \int_{\mathbb{R}} \frac{\delta H}{\delta f}\{\varphi'(f), f\}\mathrm{d}x\mathrm{d}v = 0,$$

owing to the fact that $\{\varphi'(f), f\} = 0$ for all functions φ and f. Hence the functionals (2.3) are invariant under any dynamics of the form (2.1) and they are the Casimirs invariants of the Poisson structure (compare (1.5)).

Finally, we note that owing to the expression of the Fréchet derivatives of T and U, the evolution equation (2.1) associated with these functionals corresponds to the equations (1.6). In particular, their flow can be calculated explicitely and they preserve the Casimir invariants.

2.2 Relations between T and U

The aim of this subsection is to prove the following result:

Proposition 2.1 *The functionals $T[f]$ and $U[f]$ satisfy the relation*

$$\{\{T, U\}_f, U\}_f = 2U$$

with the Poisson bracket defined in (2.2)*. In particular, the RKN identity* (1.10) *holds.*

Proof. First, we calculate the following

$$\{T,U\}_f = \frac{1}{L}\int_0^L\int_{\mathbb{R}} \frac{\delta T}{\delta f}\{\frac{\delta U}{\delta f}, f\}\mathrm{d}x\mathrm{d}v = \frac{1}{L}\int_0^L\int_{\mathbb{R}} \frac{v^2}{2}\{\phi[f], f\}\mathrm{d}x\mathrm{d}v$$
$$= -\frac{1}{L}\int_0^L\int_{\mathbb{R}} \phi[f]\{\frac{v^2}{2}, f\}\mathrm{d}x\mathrm{d}v.$$

Hence we can write

$$\{T,U\}_f = \frac{1}{L}\int_0^L\int_{\mathbb{R}} \phi[f](x)v\partial_x f(x,v)\mathrm{d}x\mathrm{d}v.$$

Let us calculate the Fréchet derivative of this functional. To this aim, we evaluate this functional at $f+\delta f$ with $\frac{1}{L}\int_0^L\int_{\mathbb{R}}\delta f = 0$. First, we have

$$\phi[f+\delta f](x) = \phi[f](x) - \partial_{xx}^{-1}\int_{\mathbb{R}} \delta f(x,w)\mathrm{d}w + \mathcal{O}(\delta f^2).$$

Hence, we have

$$\{T,U\}_{f+\delta f} = \{T,U\}_f + \frac{1}{L}\int_0^L\int_{\mathbb{R}} \phi[f](x)v\partial_x\delta f(x,v)\mathrm{d}x\mathrm{d}v$$
$$-\frac{1}{L}\int_0^L\int_{\mathbb{R}} \Big(\partial_{xx}^{-1}\int_{\mathbb{R}}\delta f(x,w)\mathrm{d}w\Big)v\partial_x f(x,v)\mathrm{d}x\mathrm{d}v + \mathcal{O}(\delta f^2).$$

We see that the third term can be written using an integration by part in x

$$-\frac{1}{L}\int_0^L\int_{\mathbb{R}} \Big(\int_{\mathbb{R}}\delta f(x,v)\mathrm{d}v\Big)v\partial_{xx}^{-1}(\partial_x f(x,v))\mathrm{d}x\mathrm{d}v.$$

The variations can only be done in the x variable. We deduce that

$$\begin{aligned}\frac{\delta\{T,U\}_f}{\delta f}[f] &= -v\partial_x\phi[f](x) - \int_{\mathbb{R}} v\partial_{xx}^{-1}(\partial_x f(x,v))\mathrm{d}v\\ &=: vE[f](x) + Z[f](x).\end{aligned}$$

Now we calculate using the previous relations that

$$\begin{aligned}\{\{T,U\}_f,U\}_f &= \frac{1}{L}\int_0^L\int_{\mathbb{R}}(Z[f](x)+vE[f](x))\{\phi[f](x), f(x,v)\}\ \mathrm{d}x\mathrm{d}v\\ &= \frac{1}{L}\int_0^L\int_{\mathbb{R}}(Z[f](x)+vE[f](x))\partial_x\phi[f](x)\partial_v f(x,v)\mathrm{d}x\mathrm{d}v.\end{aligned}$$

Now we see that the term involving the function $Z[f](x)$ vanishes, as the integral of $\partial_v f(x,v)$ in $v\in\mathbb{R}$ is equal to 0. We can thus write

$$\begin{aligned}\{\{T,U\}_f,U\}_f &= -\frac{1}{L}\int_0^L\int_{\mathbb{R}} E[f](x)^2 v\partial_v f(x,v)\mathrm{d}x\mathrm{d}v\\ &= \frac{1}{L}\int_0^L E[f](x)^2\Big(\int_{\mathbb{R}} f(x,v)\mathrm{d}v\Big)\mathrm{d}x.\end{aligned}$$

But we have

$$\int_{\mathbb{R}} f(x,v)\mathrm{d}v = 1 + \partial_x E[f](x),$$

hence

$$\begin{aligned}\{\{T,U\}_f,U\}_f &= \frac{1}{L}\int_0^L E[f](x)^2\mathrm{d}x + \frac{1}{3L}\int_0^L \partial_x\big(E[f](x)^3\big)\mathrm{d}x \\ &= \frac{1}{L}\int_0^L E[f](x)^2\mathrm{d}x = 2U[f],\end{aligned}$$

using the expression of E and U. This implies the statement. Note that this relation automatically implies (1.10). ∎

3 Statement of the results

Let us consider the characteristics of the Vlasov-Poisson system given by (1.11) and (1.12). The Taylor expansion of the *backward* characteristics around $h = 0$ is written

$$X(0;\Delta t,x,v) = \sum_{i=0}^{d} X_b^{[i]}\frac{\Delta t^i}{i!} + O(\Delta t^{d+1}),\ V(0;\Delta t,x,v) = \sum_{i=0}^{d} V_b^{[i]}\frac{\Delta t^i}{i!} + O(\Delta t^{d+1}),$$

with

$$X_b^{[i]} = \partial_h^i X(0;0,x,v),\ V_b^{[i]} = \partial_h^i V(0;0,x,v),\ i = 0,\dots,d.$$

Similarly, the Taylor expansion of the *forward* characteristics around $t = 0$ is written

$$X(\Delta t;0,x,v) = \sum_{i=0}^{d} X_f^{[i]}\frac{\Delta t^i}{i!} + O(\Delta t^{d+1}),\ V(0;\Delta t,x,v) = \sum_{i=0}^{d} V_f^{[i]}\frac{\Delta t^i}{i!} + O(\Delta t^{d+1}),$$

with

$$X_f^{[i]} = \partial_t^i X(0;0,x,v),\ V_f^{[i]} = \partial_t^i V(0;0,x,v),\ i = 0,\dots,d.$$

Note that, since the system is non autonomous, we may not have

$$Z(0,\Delta t,x,v) = Z(-\Delta t,0,x,v),\ \text{for } Z \in \{X,Y\},$$

so that the forward coefficients $Z_f^{[i]}$ and the backward coefficients $Z_b^{[i]}$, with $Z \in \{X,Y\}$, may not satisfy $Z_b^{[i]} = (-1)^i Z_f^{[i]}$.

We define the momenta

$$I_k(x) = \int_{\mathbb{R}} v^k f_0(x,v)\mathrm{d}v, \quad k = 0,\dots,d, \tag{3.1}$$

and $\overline{I}_1 = \frac{1}{L}\int_0^L I_1(y)dy$.

We then can express the time derivatives of the electric field and of the characteristics in terms of the momenta (3.1). Note that some of these computations have recently been done in [11], [6], [12] for deriving Cauchy-Kovalevsky schemes. The expressions are given in the following three lemmas.

Lemma 3.1 *The first three derivatives of the electric field are given by*

$$\partial_x E(0,x) = I_0(x) - 1,$$
$$\partial_t E(0,x) = -I_1(x) + \overline{I}_1,$$
$$\partial_t^2 E(0,x) = \partial_x I_2(x) - E(0,x)I_0(x),$$
$$\partial_t^3 E(0,x) = -\partial_x^2 I_3(x) + 3\partial_x(E(0,x)I_1(x)) + I_1(x) - \overline{I}_1 I_0(x).$$

Remark 3.2 *The previous expressions have already been obtained and used in [12]; it permits to have a third order estimate of the time dependent electric field and to get a fourth order scheme without having to electric field only once per time step.*

Lemma 3.3 *The first coefficients for the forward characteristics are given by*

$$X_f^{[0]} = x,\ X_f^{[j]} = V_f^{[j-1]},\ j = 1, \ldots, d,$$
$$V_f^{[0]} = v,\ V_f^{[1]} = E(0,x),$$
$$V_f^{[2]} = v(I_0(x) - 1) - I_1(x) + \overline{I}_1,$$
$$V_f^{[3]} = v^2 \partial_x I_0(x) - E(0,x) + \partial_x I_2(x) - 2v\partial_x I_1(x),$$
$$V_f^{[4]} = -\partial_x^2 I_3(x) + 3v\partial_x^2 I_2(x) - 3v^2\partial_x^2 I_1(x) + v^3\partial_x^2 I_0(x),$$
$$+ (I_0(x) - 1)(3(I_1(x) - vI_0(x)) + v(I_0(x) - 1) - \overline{I}_1).$$

Remark 3.4 *The formulas for the forward characteristics have been used for the order* 3 *to derive a forward semi-Lagrangian scheme (FSL-CK3) in [6, 11]. Here the formulas are also given for the order* 4*, which permits to implement a FSL-CK4 scheme.*

Lemma 3.5 *The first coefficients for the backward characteristics are given by*

$$X_b^{[0]} = x,\ X_b^{[1]} = -v,\ X_b^{[2]} = E(0,x),$$
$$X_b^{[3]} = -v(I_0(x) - 1) + 2(-I_1(x) + \overline{I}_1),$$
$$V_b^{[0]} = v,\ V_b^{[1]} = -E(0,x),$$
$$V_b^{[2]} = v(I_0(x) - 1) + I_1(x) - \overline{I}_1,$$
$$V_b^{[3]} = -v^2\partial_x I_0(x) + E(0,x) - \partial_x I_2(x) - v\partial_x I_1(x),$$
$$X_b^{[4]} = 3\partial_x I_2 - 3E(0,x)I_0 + 6v\partial_x I_1 + 3v^2\partial_x I_0 + (3E(0,x) - 2v)(I_0 - 1) - 6(I_1 - \overline{I}_1),$$
$$V_b^{[4]} = -3(I_0 - 1)(-I_1 + \overline{I}_1) + v(I_0 - 1)^2 + v^3\partial_x^2 I_0 + v^2\partial_x^2 I_1$$
$$-(-\partial_x^2 I_3 + 3E(0,x)\partial_x I_1 + 3(I_0 - 1)(I_1 - \overline{I}_1) + (I_1 - \overline{I}_1) + 2\overline{I}_1(I_0 - 1))$$
$$+ E(0,x)\partial_x I_1 + 3vE(0,x)\partial_x I_0 + v(\partial_x^2 I_2 - (I_0 - 1)I_0 - E(0,x)\partial_x I_0).$$

Remark 3.6 *From these expressions, we can obtain the CK3 and CK4 scheme for a backward semi-Lagrangian method. We thus see in this context that such schemes are not restricted to use a forward method. The computational cost is similar, the formula are just slightly modified. We have given a formula for the fourth order derivative, but it will not be useful for getting the order conditions.*

We then consider a Taylor expansion of the forward numerical characteristics:

$$X_s(\Delta t, 0, x, v) = \sum_{i=0}^{d} X_{s,f}^{[i]} \frac{\Delta t^i}{i!} + O(\Delta t^{d+1}),\ V_s(\Delta t, 0, x, v) = \sum_{i=0}^{d} V_{s,f}^{[i]} \frac{\Delta t^i}{i!} + O(\Delta t^{d+1}), \tag{3.2}$$

with

$$X_{s,f}^{[i]} = \partial_t^i X_s(0; 0, x, v),\ V_{s,f}^{[i]} = \partial_t^i V_s(0; 0, x, v),\ i = 0, \dots, d.$$

The splitting scheme will be of order $\geq d$, if the forward numerical characteristics coincide with the forward (continuous) characteristics up to order d, that is

$$X_{s,f}^{[i]} = X_f^{[i]},\ V_{s,f}^{[i]} = V_f^{[i]},\ i = 0, \dots, d. \tag{3.3}$$

We recall that a splitting scheme of $2s+1$ stages for the Vlasov equation is defined through the coefficients $a_k,\ k = 1, \dots, 2s+1$ by (1.14). The objective is to compute the relations that the coefficients should satisfy in order to obtain a fourth order scheme in time. To do that we first compute the time derivatives of the numerical electric fields; then the derivatives of the numerical characteristics ca be determined and identified with the continuous one in Lemma 3.3.

Lemma 3.7 *For $p = 0, \dots, s-1$, the first derivatives of the numerical electric field for the splitting scheme (1.14) are given by*

$$\partial_t E[g_{2p+1}](0, x) = -\sum_{k=0}^{p} a_{2k}(I_1(x) - \overline{I}_1),$$

$$\partial_t^2 E[g_{2p+1}](0, x) = \left(\sum_{k=0}^{p} a_{2k}\right)^2 \partial_x I_2(x) - 2\sum_{k=0}^{p} a_{2k} \sum_{\ell=0}^{k-1} a_{2\ell+1} E_0(x) I_0(x),$$

$$\partial_t^3 E[g_{2p+1}](0, x) = -\left(\sum_{\ell=0}^{p} a_{2\ell}\right)^3 \partial_x^2 I_3(x)$$

$$+ 6\sum_{r=1}^{p} a_{2r-1} \sum_{m=r}^{p} a_{2m} \left(\sum_{\ell=0}^{p} a_{2\ell}\partial_x(E(0, x)I_1(x)) + \sum_{\ell=0}^{r-1} a_{2\ell}(I_1(x) - \overline{I}_1 I_0(x))\right).$$

where g_{2p+1} is the function defined in (1.7).

Remark 3.8 *The quantity $\partial_t E[g_{2p+1}](0, x)$ does not lead generally to a third order approximation of the intermediate electric field $E(\sum_{j=0}^{p} a_{2j+1}\Delta t, x)$. Only after a whole time step, we get the good approximation of the characteristics. This contrast to [12], where is used a third order approximation of the intermediate electric field, which can be obtained from Lemma 3.1.*

Lemma 3.9 *The derivatives of the forward numerical characteristics (3.2) for the splitting scheme of arbitrary number of stages $2s+1$ are given by the following expressions:*

$$X_{f,s}^{[0]} = x,\ V_{f,s}^{[0]} = v,\ X_{f,s}^{[1]} = \sum_{\ell=0}^{s} a_{2\ell} v, \quad \textit{and} \quad V_{f,s}^{[1]} = \sum_{\ell=1}^{s} a_{2\ell-1} E(0, x),$$

for the zero and first orders,

$$X_{f,s}^{[2]} = 2\sum_{\ell=0}^{s} a_{2\ell} \sum_{p=1}^{\ell} a_{2p-1} E(0,x),$$
$$V_{f,s}^{[2]} = 2\sum_{\ell=1}^{s} a_{2\ell-1} \sum_{r=0}^{\ell-1} a_{2r}(v(I_0(x)-1) + \overline{I}_1 - I_1(x)),$$

for the second order,

$$X_{f,s}^{[3]} = 6\sum_{\ell=0}^{s} a_{2\ell} \sum_{p=1}^{\ell} a_{2p-1} \sum_{r=0}^{p-1} a_{2r}(\overline{I}_1 - I_1(x) + v(I_0(x)-1)),$$
$$V_{f,s}^{[3]} = 3\sum_{\ell=1}^{s} a_{2\ell-1}\times$$
$$\left(\left(\sum_{k=0}^{\ell-1} a_{2k}\right)^2 (\partial_x I_2(x) + v^2\partial_x I_0(x) - 2v\partial_x I_1(x)) - 2\sum_{p=0}^{\ell-1} a_{2p} \sum_{r=1}^{p} a_{2r-1} E(0,x)\right),$$

for the third order, and

$$X_{f,s}^{[4]} = 12\sum_{\ell=0}^{s} a_{2\ell} \sum_{q=1}^{\ell} a_{2q-1} \left(\sum_{k=0}^{q-1} a_{2k}\right)^2 (\partial_x I_2(x) + v^2\partial_x I_0(x) - 2v\partial_x I_1(x))$$
$$- 24\sum_{\ell=0}^{s} a_{2\ell} \sum_{q=1}^{\ell} a_{2q-1} \sum_{p=0}^{q-1} a_{2p} \sum_{r=1}^{p} a_{2r-1} E(0,x),$$

$$V_{f,s}^{[4]} = 4\sum_{\ell=1}^{s} a_{2\ell-1} \left(\sum_{k=0}^{\ell-1} a_{2k}\right)^3 \left(-\partial_x^2 I_3(x) + 3\partial_x^2 I_2(x)v - 3v^2\partial_x^2 I_1(x) + v^3\partial_x^2 I_0(x)\right)$$
$$+ 24\sum_{\ell=1}^{s} a_{2\ell-1} \sum_{r=1}^{\ell-1} a_{2r-1} \sum_{m=r}^{\ell-1} a_{2m} \sum_{q=0}^{\ell-1} a_{2q}(I_0(x)-1)(I_1(x) - vI_0(x))$$
$$+ 24\sum_{\ell=1}^{s} a_{2\ell-1} \sum_{r=1}^{\ell-1} a_{2r-1} \sum_{m=r}^{\ell-1} a_{2m} \sum_{q=0}^{r-1} a_{2q}(I_0(x)-1)((I_0(x)-1)v - \overline{I}_1).$$

for the fourth order.

To compute the coefficients $a_j, j = 0, \ldots, 2s+1$, we have to identify the time derivatives of continuous and numerical forward characteristics. From Lemmas 3.3 and 3.9, we see that the forward numerical and continuous characteristic expansions are expressed with the same terms (depending on momenta $I_k, k = 0, \ldots, 3$ of f and on $E(0,x)$). This permits to derive the order conditions.

As in [2], we introduce the coefficients p_j which enable to make the link with the PRK and RKN methods

$$p_0 = 0, \; p_{j+1} = a_j - p_j, \quad j = 0, \dots, 2s,$$

together with

$$B_1 = \sum_{j=1}^{2s} p_j, \qquad B_2 = \sum_{j=1}^{2s} (-1)^j p_j^2,$$
$$B_{4a} = \sum_{j=1}^{2s} (-1)^j p_j^4, \quad B_{4b} = \sum_{j=1}^{s} (p_{2j}^3 + p_{2j-1}^3) \sum_{k=1}^{2j-1} p_k,$$
$$B_{4c} = \sum_{j=1}^{s} (p_{2j}^2 - p_{2j-1}^2) \left(\sum_{k=1}^{j-1} p_{2k} \sum_{\ell=1}^{2k-1} p_\ell + \sum_{k=1}^{j} p_{2k-1} \sum_{\ell=1}^{2k-1} p_\ell \right).$$

Thanks to all the previous identities, we obtain the order conditions for the fourth order in a reduced form.

Theorem 3.10 *The conditions on $p_j, j = 1, \dots, 2s+1$ which ensures that the time splitting of arbitrary stages $2s+1$ is fourth order (i.e. (3.3)), can be rewritten as*

$$p_{2s+1} = 0, \; B_1 = 1, \tag{3.4}$$
$$B_2 = 0, \tag{3.5}$$
$$B_{3a} = B_{3b} = 0, \tag{3.6}$$
$$B_{4a} = -4B_{4b} = 4B_{4c}, \tag{3.7}$$

as soon as we assume that the following functions inside the brackets are independent: $[vI_0(x) - 1, I_1(x) - \overline{I}_1]$, $[\partial_x I_2(x) + v^2 \partial_x I_0(x) - 2v\partial_x I_1(x), E(0,x)]$ *and*

$$[-\partial_x^2 I_3(x) + 3\partial_x^2 I_2(x) v - 3v^2 \partial_x^2 I_1(x) + v^3 \partial_x^2 I_0(x),$$
$$(I_0(x) - 1)(I_1(x) - vI_0(x)), (I_0(x) - 1)((I_0(x) - 1)v - \overline{I}_1)].$$

The proof of this result is postponed to 5.

Remark 3.11 *More precisely, (3.4) corresponds for the first order, (3.4)-(3.5) to the second order and (3.4)-(3.5)-(3.6) to the third order. We thus get the same conditions as the PRK methods presented in Blanes et al. [2] for order ≤ 3 and as RKN for the order 4 (for order ≤ 3, the coefficients for the PRK methods coincide with the coefficients of the RKN methods).*

4 Numerical results

We consider the non linear Landau damping test case for which the initial condition writes

$$f_0(x, v) = \frac{1}{\sqrt{2\pi}} \exp(-v^2/2)(1 + \alpha \cos(kx)),$$

with

$$N_x = N_v = 1024,\ \Delta t = 0.125,\ v_{\max} = 6,\ k = 0.5,\ \alpha = 0.5,$$

and take Lagrange interpolation of order 17 in the spatial direction ($x \in [0, 2\pi/k]$) and in the velocity direction ($v \in [-v_{\max}, v_{\max}]$), see *e.g.* [5, 1, 4, 7]. The coefficients that we use can be found in the literature (see *e.g.* [3],[2]); the first digits are given here for convenience. We will here also consider splitting schemes that begin with a v-advection: $g_1(x, v) = f_0(x, v - b_0\, E[g_0](x)\, \Delta t)$, and

$$\begin{aligned} g_{2j}(x, v) &= g_{2j-1}(x - b_{2j-1}\, v\, \Delta t, v), \\ g_{2j+1}(x, v) &= g_{2j}(x, v - b_{2j}\, E[g_{2j}](x)\, \Delta t), \end{aligned} \tag{4.1}$$

for $j = 1, \ldots, 2s$. Note that such a scheme can be recasted in a scheme of the form (1.7), by taking $a_0 = a_{2s+2} = 0,\ a_j = b_{j-1},\ j = 1, \ldots, 2s + 1$.

- **Strang (s=1)**:
$[a_0, a_2] = [0.5, 0.5],\ a_1 = 1.$
- **Strang v-x (s=1)**:
$[b_0, b_2] = [0.5, 0.5],\ b_1 = 1.$
- **Triple jump (s=3)**:
$[a_0, a_2, a_4, a_6] = [0.676, -0.176, -0.176, 0.676],$
$[a_1, a_3, a_5] = [1.351, -1.70, 1.35].$
- **Order 4 (s=6)**:
$[b_0, b_2, \ldots, b_{12}] = [0.0830, 0.396, -0.0391, 0.120, -0.0391, 0.396, 0.0830],$
$[b_1, b_3, \ldots, b_{11}] = [0.245, 0.605, -0.350, -0.350, 0.605, 0.245].$
- **Order 6 (s=11)**:
$[b_0, b_2, \ldots, b_{22}] = [0.0415, 0.198, -0.04, 0.0753, -0.0115, 0.237,$
$0.237, -0.0115, 0.0753, -0.04, 0.198, 0.0415],$
$[b_1, b_3, \ldots, b_{21}] = [0.123, 0.291, -0.127, -0.246, 0.357, 0.205,$
$0.357, -0.246, -0.127, 0.291, 0.123].$

For these different splittings, we plot on Figures 1 and 2 the time history of the electric energy $\mathcal{E}_e(t) = \int_0^{2\pi/k} E(t, x)^2 dx$, the total energy $\mathcal{E}(t)$ defined as

$$\mathcal{E}(t) = \int_{\mathbb{R}} \int_0^{2\pi/k} v^2 f(t, x, v) dx dv + \mathcal{E}_e(t),$$

and the $L^p, p = 1, 2$ norms of f. Let us recall that the total energy and L^p norms are conserved quantities of the model. The diagnostic of the electric energy does not present significative difference, but the behaviour is in good agreement with results of the literature [5]. The same is true for the $L^p, p = 1, 2$ norms of f since no real impact of high order splittings can be seen on the evolution of these quantities (which essentially depends on the spatial and velocity discretization). However, we clearly see in Figure 1 the advantage of using high order schemes in time for the energy conservation; this was already pointed out in [15], but the optimized coefficients of Blanes and Moan [3] give even better results. We have also tried the coefficients of order 10 given in [14] which do not improve the order 6 results in our testcase. On these figures, we plot the Strang splitting with a time step divided by 20 ("strang $v - x$ $dt/20$"): the time of the simulation is then the same between "strang $v - x$ $dt/20$" scheme (brown curve) and "order $6 s = 11$" scheme (light blue curve). For a given time simulation, we then emphasize the fact that the high order splitting with optimized coefficients gives the best results in our case.

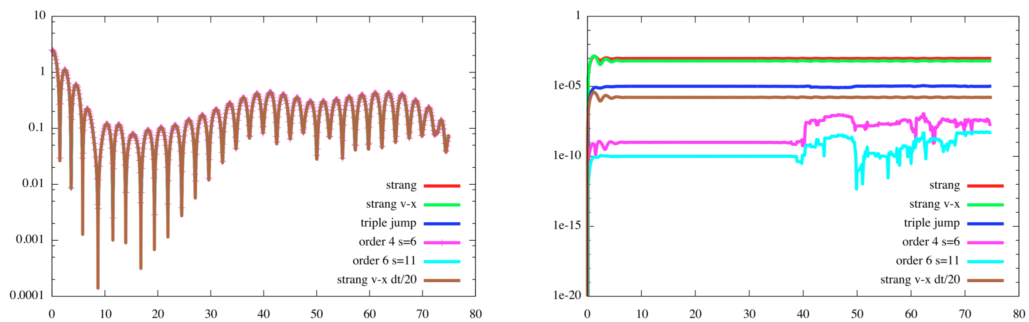

Figure 1: Time history of the electric energy (left) and of the total energy (right), for the different time splitting algorithms.

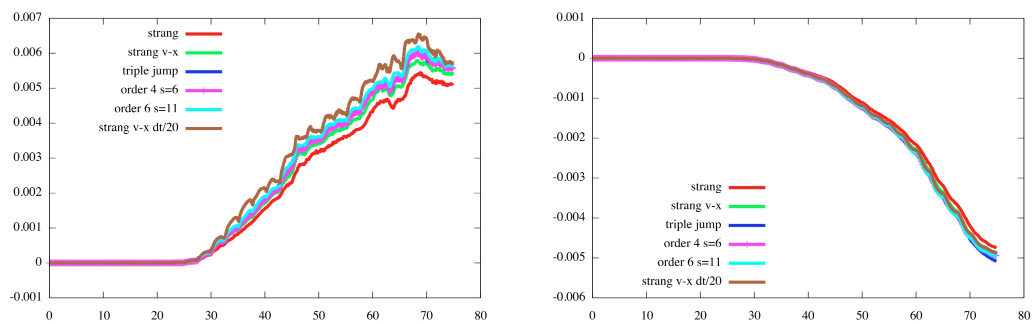

Figure 2: Time history of the L^1 norm of f (left) and of the L^2 norm of f (right), for the different time splitting algorithms.

5 Proof of the results

This section is devoted to the proof of Lemma 3.9. We then also give the equations that have to be satisfied by identifying with the Taylor expansion of the continuous characteristics derived in Lemma 3.3.

5.1 The strategy

5.1.1 Expansion of a unified form of the splitting

The following result will be used for the expansions of backward and forward numerical characteristics.

Proposition 5.1 *For all $j \geq 0$, assume that $G_{2j+1}(t,x)$ are given functions with Taylor expansion*

$$G_{2j+1}(t,x) = \sum_{k\geq 0} \frac{t^k}{k!} g^k_{2j+1}(x)$$

around $t = 0$, where $g_{2j+1}(x)$ are given functions of x. For $(x,v) \in [0,L] \times \mathbb{R}$, and sufficiently small t, we define the functions $Z_j(t,x,v)$ and $W_j(t,x,v)$ by the relations

$$Z_0(t,x,v) = x, W_0(t,x,v) = v, \tag{5.1}$$

$$Z_{j+1}(t,x,v) = Z_j(t,x,v) + c_{2j} t W_j(t,x,v), \quad j \geq 0 \tag{5.2}$$

$$W_{j+1}(t,x,v) = W_j(t,x,v) + c_{2j+1} t G_{2j+1}(t, Z_{j+1}(t,x,v)), \quad j \geq 0 \tag{5.3}$$

for $j \geq 0$. Denoting by $z^k_j(x,v) = \partial^k_t Z_j(0,x,v)$ and $w^k_j(x,v) = \partial^k_t W_j(0,x,v)$, then the following relations hold true:

$$z^0_j(x;v) = x, \ w^0_j(x,v) = v, \ j \geq 0$$

and for $r = 1, \dots, 4$ and $j \geq 0$

$$z^r_{j+1}(x,v) = r\sum_{\ell=0}^{j} c_{2\ell} w^{r-1}_\ell(x,v) \ \ \text{and} \ \ w^r_j(x,v) = r\sum_{\ell=1}^{j} c_{2\ell-1}\mathcal{E}^r_\ell(x,v), \tag{5.4}$$

with

$$\mathcal{E}^1 = g^0, \ \mathcal{E}^2 = g^1 + z^1\partial_x g^0, \ \mathcal{E}^3 = g^2 + 2z^1\partial_x g^1 + (z^1)^2\partial^2_x g^0 + z^2\partial_x g^0$$
$$\mathcal{E}^4 = g^3 + 3z^1\partial_x g^2 + 3(z^1)^2\partial^2_x g^1 + 3z^2\partial_x g^1 + (z^1)^3\partial^3_x g^0 + 3z^1z^2\partial^2_x g^0 + z^3\partial_x g^0.$$

The proof of this Proposition is straightforward using Taylor expansions. Such relations permit to compute the sequences by induction. For $r = 1$, we obtain

$$z^1_{j+1} = \sum_{\ell=0}^{j} c_{2\ell} v, \ w^1_j = \sum_{\ell=1}^{j} c_{2\ell-1} g^0_\ell, \ j = 0, \dots \tag{5.5}$$

For $r = 2$, we obtain

$$z^2_{j+1} = 2\sum_{k=0}^{j} c_{2k} w^1_k = 2\sum_{k=0}^{j} c_{2k} \sum_{\ell=1}^{k} c_{2\ell-1} g^0_\ell, \tag{5.6}$$

and

$$w^2_{j+1} = 3\sum_{k=0}^{j} c_{2k-1} g^1_k + 3\sum_{k=0}^{j} c_{2k-1} z^1_k \partial_x g^0_k = 3\sum_{k=0}^{j} c_{2k-1} g^1_k + 3\sum_{k=0}^{j} c_{2k-1} \sum_{\ell=0}^{k-1} c_{2\ell} v \partial_x g^0_k. \tag{5.7}$$

5.1.2 Derivatives of the electric field

For the computation of the derivatives of the electric field, we introduce

$$E[\psi, Z, W](t,x) = \int_0^L K(x,y) \int_{\mathbb{R}} \psi(Z(t,y,v), W(t,y,v))\mathrm{d}v\mathrm{d}y,$$

where $\psi(x,v)$, $Z(t,x,v)$ and $W(t,x,v)$ are given functions. The Taylor expansion of $E[\psi, Z, W]$ can be computed using the following result, whose proof is again a identification of Taylor expansions around $t = 0$:

Proposition 5.2 *Let $\mathcal{Z}^k(y,v) = \partial_t^k Z(0,y,v)$ and $\mathcal{W}^k(y,v) = \partial_t^k W(0,y,v)$. Then the following relations hold true for $k = 0, \ldots, 3$*

$$\partial_t^k E[\psi, Z, W](0,x) = \int_0^L K(x,y) \int_{\mathbb{R}} \phi^k(y,v)\mathrm{d}v\mathrm{d}y, \tag{5.8}$$

with

$$\phi^0 = \psi, \phi^1 = \mathcal{Z}^1\partial_x\psi + \mathcal{W}^1\partial_v\psi$$
$$\phi^2 = \mathcal{Z}^2\partial_x\psi + (\mathcal{Z}^1)^2\partial_x^2\psi + 2\mathcal{Z}^1\mathcal{W}^1\partial_x\partial_v\psi + \mathcal{W}^2\partial_v\psi + (\mathcal{W}^1)^2\partial_v^2\psi$$

and

$$\begin{aligned}\phi^3 = {}& \mathcal{Z}^3\partial_x\psi + 3\mathcal{Z}^1\mathcal{Z}^2\partial_x^2\psi + 3\mathcal{Z}^2\mathcal{W}^1\partial_x\partial_v\psi + (\mathcal{Z}^1)^3\partial_x^3\psi + 3(\mathcal{Z}^1)^2\mathcal{W}^1\partial_x^2\partial_v\psi \\ & + 3\mathcal{Z}^1\mathcal{W}^2\partial_x\partial_v\psi + 3\mathcal{Z}^1(\mathcal{W}^1)^2\partial_x\partial_v^2\psi + \mathcal{W}^3\partial_v\psi + 3\mathcal{W}^1\mathcal{W}^2\partial_v^2\psi + (\mathcal{W}^1)^3\partial_v^3\psi.\end{aligned}$$

5.1.3 Backward characteristics for the electric field

Let $p \in \{0, \ldots, s-1\}$, and let g_{2p+1} be the functions defined in (1.7). We consider the following quantities

$$E_{2p+1}(t,x) := E[g_{2p+1}](t,x) = \int_0^L K(x,y) \int_{\mathbb{R}} f(0, X_{p+1}^b(t,y,v), V_p^b(t,y,v))\mathrm{d}y\mathrm{d}v, \tag{5.9}$$

for which we have to compute the successive derivatives in time, for $t = 0$. Here $X_{p+1}^b(t,y,v)$ and $V_p^b(t,y,v)$ are backward numerical characteristics obtained from the splitting scheme until the stage $2p+1$. More precisely, we take the following specialization in (5.1)-(5.3)

$$c_0 = -a_{2p},\ c_1 = -a_{2p-1},\ \ldots, c_{2p} = -a_0$$

and the functions

$$G_1 = E_{2p-1},\ \ldots, G_{2p-1} = E_1,$$

so that

$$X_{p+1}^b(t,x,v) = Z_{p+1}(t,x,v),\ V_p^b(t,x,v) = W_p(t,x,v). \tag{5.10}$$

We can then compute the successive derivatives

$$\partial_t^r X_{p+1}^b(0,x,v),\ \partial_t^r V_p^b(0,x,v),\ \partial_t^r E_{2p+1}(0,x),\ r=0,\dots,3,$$

by using Propositions 5.1 and 5.2. In the following we fix the notations $z_{p+1}^r = \partial_t^r Z_{p+1}(0,x,v)$ and $w_p^r = \partial_t W_p(0,x,v)$ defined in (5.10) and in Proposition 5.1. Moreover, for $p=0,\dots,s-1$, we define the functions ϕ_{2p+1}^k by the formula

$$\partial_t^k E_{2p+1}(0,x) = \int_0^L K(x,y)\int_{\mathbb{R}} \phi_{2p+1}^k(y,v)\mathrm{d}v\mathrm{d}y,$$

compare (5.8).

5.1.4 Forward characteristics

Once we have computed such derivatives, we can consider the forward numerical characteristics.
We take $c_j = a_j,\ j=0,\dots,2s,\ G_{2j+1}=E_{2j+1},\ j=0,\dots,s-1$ in (5.1)-(5.3) and the forward numerical characteristics are given by

$$X_{s+1}^f(t,x,v) = Z_{s+1}(x,v),\ V_s^f(t,x,v) = W_s(x,v).$$

We are then able to give expressions of

$$\partial_t^r X_{s+1}^f(0,x,v) = \partial_t^r Z_{s+1}(0,x,v),\ \partial_t^r V_s^f(0,x,v) = \partial_t^r W_s(0,x,v),$$

for $r=0,\dots,4$, by applying Proposition 5.1 and the expression of the derivatives of the electric field obtained with the backward characteristics. Again, we fix the notations $z_{s+1}^r = \partial_t^r Z_{s+1}(0,x,v)$ and $w_p^r = \partial_t W_s(0,x,v)$ defined above.

5.2 Time derivatives of the electric field

Note that using (5.9), we have $E_{2p+1}(0,x) = E(0,x)$ for all $p=0,\dots,s-1$. We also set $E_0(x) := E(0,x)$.

5.2.1 Computation of the first derivative of E_{2p+1}

Using Proposition 5.1, we have for all $p=0,\dots,s-1$,

$$\partial_t V_p^b(0,x,v) = w_p^1 = -\sum_{\ell=1}^p a_{2\ell-1}E_0(x),\ \partial_t X_{p+1}^b(0,x,v) = z_{p+1}^1 = -\sum_{\ell=1}^p a_{2\ell} v,$$

from which we can compute $\phi_{2p+1}^1 = z_{p+1}^1\partial_x f_0 + w_p^1\partial_v f_0$, in order to finally get

$$g_{p+1}^1 = \partial_t E_{2p+1}(0,x) = \int_0^L K(x,y)\int \phi_{2p+1}^1(y,v)dv = -\sum_{\ell=0}^p a_{2\ell}(I_1(x)-\overline{I}_1).$$

5.2.2 Computation of the second derivative of E_{2p+1}

Similarly, we have for $p = 0, \dots, s-1$

$$\partial_t^2 X_{p+1}^b(0,x,v) = z_{p+1}^2 = 2\sum_{k=0}^{p-1} a_{2k} \sum_{\ell=k}^{p-1} a_{2\ell+1} E(0,x),$$

and

$$\partial_t^2 V_p^b(0,x,v) = w_p^2 = 2\sum_{k=1}^{p} a_{2k-1} \sum_{\ell=0}^{k-1} a_{2\ell}(I_1 - \overline{I}_1) + 2\sum_{k=1}^{p} a_{2k-1} \sum_{\ell=k}^{p} a_{2\ell} v \partial_x E(0,x).$$

We can then compute

$$\phi_{2p+1}^2 = z_{p+1}^2 \partial_x f_0 + (z_{p+1}^1)^2 \partial_x^2 f_0 + 2 z_{p+1}^1 w_p^1 \partial_x \partial_v f_0 + w_p^2 \partial_v f_0 + (w_p^1)^2 \partial_v^2 f_0$$

and get

$$\int \phi_{2p+1}^2 \mathrm{d}v = \left(\sum_{k=0}^{p} a_{2k}\right)^2 \partial_x^2 I_2 - 2\sum_{k=0}^{p} a_{2k} \sum_{\ell=0}^{k-1} a_{2\ell+1} \partial_x (E_0 I_0),$$

where we use the identity $\sum_{k=0}^{p}\sum_{\ell=0}^{k-1} a_{2k} a_{2\ell+1} = \sum_{k=1}^{p} a_{2k-1} \sum_{\ell=k}^{p} a_{2\ell}$. We deduce that

$$g_{p+1}^2 = \partial_t^2 E_{2p+1}(0,\cdot) = \left(\sum_{k=0}^{p} a_{2k}\right)^2 \partial_x I_2 - 2\sum_{k=0}^{p} a_{2k} \sum_{\ell=0}^{k-1} a_{2\ell+1} E_0 I_0.$$

5.2.3 Computation of the third derivative of E_{2p+1}

We have for $p = 0, \dots, s-1$,

$$\begin{aligned}
&\partial_t^3 X_{p+1}^b(0,x,v) = z_{p+1}^3 \\
&= -6\sum_{m=0}^{p-1} a_{2m+1} \left(\sum_{j=0}^{m} a_{2j}\right)^2 (I_1(x) - \overline{I}_1) - 6\sum_{m=0}^{p-1} a_{2m+1} \sum_{j=0}^{m} a_{2j} \sum_{\ell=m+1}^{p} a_{2\ell} v \partial_x E_0(x),
\end{aligned}$$

and

$$\begin{aligned}
\partial_t^3 V_p^b(0,x,v) = w_p^3 &= 3\sum_{r=1}^{p} a_{2r-1} \left(\sum_{m=0}^{r-1} a_{2m}\right)^2 \partial_x I_2(x) \\
&+ 6\sum_{r=1}^{p} a_{2r-1} \sum_{m=0}^{r-1} a_{2m} \sum_{\ell=0}^{m-1} a_{2\ell+1} (E_0 I_0)(x) - 6\sum_{r=1}^{p} a_{2r-1} \sum_{m=r}^{p} a_{2m} \sum_{\ell=0}^{r-1} a_{2\ell} v \partial_x I_1(x) \\
&- 3\sum_{r=1}^{p} a_{2r-1} \left(\sum_{m=r}^{p} a_{2m}\right)^2 v^2 \partial_x^2 E_0(x) - 6\sum_{r=1}^{p} a_{2r-1} \sum_{m=r}^{p-1} a_{2m} \sum_{\ell=j}^{p-1} a_{2\ell+1} E_0(x) \partial_x E_0(x).
\end{aligned}$$

We then get

$$\int \phi^3_{2p+1} \mathrm{d}v = A_1 E_0 \partial_x^2 I_1 + A_2 \partial_x E_0 \partial_x I_1 + A_3 \partial_x I_1 + A_4 \overline{I}_1 \partial_x I_0 + A_5 I_1 \partial_x^2 E_0,$$

with

$$\begin{aligned}
A_1 &= 6\sum_{j=1}^{p} a_{2j-1}\left(\sum_{\ell=0}^{p} a_{2\ell}\right)^2 - 6\sum_{j=0}^{p} a_{2j}\sum_{k=0}^{p-1} a_{2k}\sum_{\ell=k}^{p-1} a_{2\ell+1},\\
A_2 &= 12\sum_{j=0}^{p} a_{2j}\sum_{k=1}^{p} a_{2k-1}\sum_{\ell=k}^{p} a_{2\ell} - 6\sum_{m=0}^{p-1} a_{2m+1}\sum_{j=0}^{m} a_{2j}\sum_{\ell=m+1}^{p} a_{2\ell}\\
&\quad +6\sum_{r=1}^{p} a_{2r-1}\sum_{m=r}^{p} a_{2m}\sum_{\ell=0}^{r-1} a_{2\ell},\\
A_3 &= 6\sum_{r=1}^{p} a_{2r-1}\sum_{m=r}^{p} a_{2m}\sum_{\ell=0}^{r-1} a_{2\ell},\\
A_4 &= -6\sum_{j=0}^{p} a_{2j}\sum_{k=1}^{p} a_{2k-1}\sum_{\ell=0}^{k-1} a_{2\ell} + 6\sum_{m=0}^{p-1} a_{2m+1}\left(\sum_{j=0}^{m} a_{2j}\right)^2, \quad \text{and}\\
A_5 &= 6\sum_{j=0}^{p} a_{2j}\sum_{k=1}^{p} a_{2k-1}\sum_{\ell=0}^{k-1} a_{2\ell} - 6\sum_{m=0}^{p-1} a_{2m+1}\left(\sum_{j=0}^{m} a_{2j}\right)^2\\
&\quad +6\sum_{r=1}^{p} a_{2r-1}\left(\sum_{m=r}^{p} a_{2m}\right)^2.
\end{aligned}$$

Some relations can be exhibited between the coefficients $A_i, i = 1, \dots 5$. Indeed, we have $A_4 = -A_3$, $A_5 = A_2/2$, and $A_1 = A_2/2 = A_5$ but also

$$A_2 = 12\sum_{j=0}^{p} a_{2j}\sum_{k=1}^{p} a_{2k-1}\sum_{\ell=k}^{p} a_{2\ell}.$$

We then obtain a simplified expression

$$\int \phi^3_{2p+1} \mathrm{d}v = -\left(\sum_{\ell=0}^{p} a_{2\ell}\right)^3 \partial_x^3 I_3 + A_1 \partial_x^2 (E_0 I_1) + A_3 \partial_x (I_1 - \overline{I}_1 I_0),$$

with

$$A_1 = 6\sum_{r=1}^{p} a_{2r-1}\sum_{m=r}^{p} a_{2m}\sum_{\ell=0}^{p} a_{2\ell}, \quad \text{and} \quad A_3 = 6\sum_{r=1}^{p} a_{2r-1}\sum_{m=r}^{p} a_{2m}\sum_{\ell=0}^{r-1} a_{2\ell}.$$

Finally, we can write the third derivative of E_{2p+1}

$$g^3_{p+1} = \partial_t^3 E_{2p+1}(0,\cdot) = -\left(\sum_{\ell=0}^{p} a_{2\ell}\right)^3 \partial_x^2 I_3 + A_1 \partial_x (E_0 I_1) + A_3 (I_1 - \overline{I}_1 I_0).$$

5.3 Computation of the forward characteristics

We have at first

$$X^f_{s+1}(0,x,v) = z^0_{s+1} = x,\ \ V^f_s(0,x,v) = w^0_s = v,$$

and

$$\partial_t X^f_{s+1}(0,x,v) = z^1_{s+1} = \sum_{\ell=0}^{s} a_{2\ell} v,\ \ \partial_t V^f_s(0,x,v) = w^1_s = \sum_{\ell=1}^{s} a_{2\ell-1} E(0,x).$$

For the second derivatives, we get using Proposition 5.1

$$\partial_t^2 X^f_{s+1}(0,x,v) = z^2_{s+1} = 2\sum_{\ell=0}^{s} a_{2\ell} \sum_{p=1}^{\ell} a_{2p-1} E(0,x),$$

and

$$\begin{aligned}\partial_t^2 V^f_s(0,x,v) = w^2_s &= 2\sum_{\ell=1}^{s} a_{2\ell-1}(\partial_t E_{2\ell-1} + z^1_\ell \partial_x E_{2\ell-1}) \\ &= 2\sum_{\ell=1}^{s} a_{2\ell-1} \sum_{r=0}^{\ell-1} a_{2r}(\overline{I}_1 - I_1 + v(I_0 - 1)).\end{aligned}$$

For the third derivative, we get

$$\partial_t^3 X^f_{s+1}(0,x,v) = z^3_{s+1} = 6\sum_{\ell=0}^{s} a_{2\ell} \sum_{p=1}^{\ell} a_{2p-1} \sum_{r=0}^{p-1} a_{2r}(\overline{I}_1 - I_1 + v(I_0 - 1)).$$

and

$$\begin{aligned}\partial_t^3 V^f_s(0,x,v) = w^3_s &= 3\sum_{\ell=1}^{s} a_{2\ell-1}\left(\sum_{k=0}^{\ell-1} a_{2k}\right)^2 (\partial_x I_2 + v^2 \partial_x I_0 - 2v\partial_x I_1) \\ &\quad - 6\sum_{\ell=1}^{s} a_{2\ell-1} \sum_{p=0}^{\ell-1} a_{2p} \sum_{r=1}^{p} a_{2r-1} E_0.\end{aligned}$$

For the fourth derivative, we get

$$\begin{aligned}\partial_t^4 X^f_{s+1}(0,x,v) = z^4_{s+1} &= 12\sum_{\ell=0}^{s} a_{2\ell} \sum_{q=1}^{\ell} a_{2q-1}\left(\sum_{k=0}^{q-1} a_{2k}\right)^2 (\partial_x I_2 + v^2 \partial_x I_0 - 2v\partial_x I_1) \\ &\quad - 24\sum_{\ell=0}^{s} a_{2\ell} \sum_{q=1}^{\ell} a_{2q-1} \sum_{p=0}^{q-1} a_{2p} \sum_{r=1}^{p} a_{2r-1} E_0.\end{aligned}$$

Let us detail the computation for the last derivative. We first have from Proposition 5.1

$$\partial_t^4 V_{s+1}^f(0,x,v) = w_{s+1}^4 = 4\sum_{\ell=1}^{s} a_{2\ell-1}\mathcal{E}_\ell^4,$$

with $g_\ell^k = \partial_t^k E_{2\ell-1}(0,x), k = 0,\ldots,3$. Introducing the following quantities

$$A_{1,p} = 6\sum_{r=1}^{p} a_{2r-1}\sum_{m=r}^{p} a_{2m}\sum_{\ell=0}^{p} a_{2\ell},\ \ A_{3,p} = 6\sum_{r=1}^{p} a_{2r-1}\sum_{m=r}^{p} a_{2m}\sum_{\ell=0}^{r-1} a_{2\ell},$$

we calculate

$$\begin{aligned}
g_\ell^3 &= -\left(\sum_{k=0}^{\ell-1} a_{2k}\right)^3 \partial_x^2 I_3 + A_{1,\ell-1}\partial_x(E_0 I_1) + A_{3,\ell-1}(I_1 - \overline{I}_1 I_0),\\
3z_\ell^1\partial_x g_\ell^2 &= 3\left(\left(\sum_{k=0}^{\ell-1} a_{2k}\right)^2 \partial_x^2 I_2 - 2\sum_{k=0}^{\ell-1} a_{2k}\sum_{q=0}^{k-1} a_{2q+1}\partial_x(E_0 I_0)\right)\sum_{k=0}^{\ell-1} a_{2k} v,\\
3(z_\ell^1)^2\partial_x^2 g_\ell^1 &= -3\left(\sum_{k=0}^{\ell-1} a_{2k} v\right)^2 \sum_{k=0}^{\ell-1} a_{2k}\partial_x^2 I_1,
\end{aligned}$$

and

$$\begin{aligned}
3z_\ell^2\partial_x g_\ell^1 &= -6\left(\sum_{k=0}^{\ell-1} a_{2k}\sum_{p=1}^{k} a_{2p-1}E_0\right)\sum_{k=0}^{\ell-1} a_{2k}\partial_x I_1,\\
(z_\ell^1)^3\partial_x^3 g_\ell^0 &= \left(\sum_{k=0}^{\ell-1} a_{2k} v\right)^3 \partial_x^3 E_0,\\
3z_\ell^1 z_\ell^2\partial_x^2 g_\ell^0 &= 6\left(\sum_{k=0}^{\ell-1} a_{2k} v\right)\partial_x^2 E_0 \sum_{k=0}^{\ell-1} a_{2k}\sum_{q=1}^{k} a_{2q-1}E_0,\\
z_\ell^3\partial_x g_\ell^0 &= 6\sum_{k=0}^{\ell-1} a_{2k}\sum_{p=1}^{k} a_{2p-1}\sum_{r=0}^{p-1} a_{2r}(\overline{I}_1 - I_1 + v(I_0-1))\partial_x E_0.
\end{aligned}$$

After some calculations, we thus finally get

$$\begin{aligned}
\mathcal{E}_\ell^4 = \left(\sum_{k=0}^{\ell-1} a_{2k}\right)^3 &\left(-\partial_x^2 I_3 + 3\partial_x^2 I_2 v - 3v^2\partial_x^2 I_1 + v^3\partial_x^2 I_0\right)\\
&+ 6\sum_{r=1}^{\ell-1} a_{2r-1}\sum_{m=r}^{\ell-1} a_{2m}\sum_{q=0}^{\ell-1} a_{2q}(I_0-1)(I_1 - vI_0)\\
&\quad + 6\sum_{r=1}^{\ell-1} a_{2r-1}\sum_{m=r}^{\ell-1} a_{2m}\sum_{q=0}^{r-1} a_{2q}(I_0-1)((I_0-1)v - \overline{I}_1),
\end{aligned}$$

which enables to calculate the expression

$$\begin{aligned}\partial_t^4 V_{s+1}^f(0,x,v) = 4\sum_{\ell=1}^{s} a_{2\ell-1}\left(\sum_{k=0}^{\ell-1} a_{2k}\right)^3 \left(-\partial_x^2 I_3 + 3\partial_x^2 I_2 v - 3v^2\partial_x^2 I_1 + v^3\partial_x^2 I_0\right)\\ + 24\sum_{\ell=1}^{s} a_{2\ell-1}\sum_{r=1}^{\ell-1} a_{2r-1}\sum_{m=r}^{\ell-1} a_{2m}\sum_{q=0}^{\ell-1} a_{2q}(I_0-1)(I_1-vI_0)\\ + 24\sum_{\ell=1}^{s} a_{2\ell-1}\sum_{r=1}^{\ell-1} a_{2r-1}\sum_{m=r}^{\ell-1} a_{2m}\sum_{q=0}^{r-1} a_{2q}(I_0-1)((I_0-1)v-\overline{I}_1).\end{aligned}$$

5.4 The equations

We now summarize the equations which should be satisfied:

$$[X_1]\quad \sum_{\ell=0}^{s} a_{2\ell} = 1, \qquad [V_1]\quad \sum_{\ell=1}^{s} a_{2\ell-1} = 1,$$

and

$$[X_2]\quad 2\sum_{\ell=0}^{s} a_{2\ell}\sum_{p=1}^{\ell} a_{2p-1} = 1, \qquad [V_2]\quad 2\sum_{\ell=1}^{s} a_{2\ell-1}\sum_{r=0}^{\ell-1} a_{2r} = 1,$$

for the first and second order,

$$[X_3]\quad 6\sum_{\ell=0}^{s} a_{2\ell}\sum_{p=1}^{\ell} a_{2p-1}\sum_{r=0}^{p-1} a_{2r} = 1,$$

and

$$[V_{3a}]\quad 3\sum_{\ell=1}^{s} a_{2\ell-1}\left(\sum_{k=0}^{\ell-1} a_{2k}\right)^2 = 1, \qquad [V_{3b}]\quad 6\sum_{\ell=1}^{s} a_{2\ell-1}\sum_{p=0}^{\ell-1} a_{2p}\sum_{r=1}^{p} a_{2r-1} = 1,$$

for the third order. To get the fourth order, we get the conditions

$$[X_{4a}]\quad 12\sum_{\ell=0}^{s} a_{2\ell}\sum_{q=1}^{\ell} a_{2q-1}\left(\sum_{k=0}^{q-1} a_{2k}\right)^2 = 1,$$

$$[X_{4b}]\quad 24\sum_{\ell=0}^{s} a_{2\ell}\sum_{q=1}^{\ell} a_{2q-1}\sum_{p=0}^{q-1} a_{2p}\sum_{r=1}^{p} a_{2r-1} = 1$$

and

$$[V_{4a}]\quad 4\sum_{\ell=1}^{s} a_{2\ell-1}\left(\sum_{k=0}^{\ell-1} a_{2k}\right)^3 = 1,$$

$$[V_{4b}]\quad 8\sum_{\ell=1}^{s} a_{2\ell-1}\sum_{r=1}^{\ell-1} a_{2r-1}\sum_{m=r}^{\ell-1} a_{2m}\sum_{q=0}^{\ell-1} a_{2q} = 1,$$

$$[V_{4c}]\quad 24\sum_{\ell=1}^{s} a_{2\ell-1}\sum_{r=1}^{\ell-1} a_{2r-1}\sum_{m=r}^{\ell-1} a_{2m}\sum_{q=0}^{r-1} a_{2q} = 1.$$

The objective is to find relations between these equations to obtain a reduced system of conditions.

Order 2. We have at first $[X_2] + [V_2] = 2[X_1][V_1]$:

$$2\sum_{\ell=0}^{s} a_{2\ell} \sum_{p=1}^{\ell} a_{2p-1} + 2\sum_{p=1}^{s} a_{2p-1} \sum_{\ell=0}^{p-1} a_{2\ell} = 2\sum_{\ell=0}^{s} a_{2\ell} \sum_{p=1}^{s} a_{2p-1}.$$

Next, as in [2] we introduce

$$p_0 = 0,\ p_{j+1} = a_j - p_j,\ j = 0, \dots, 2s,$$

so that $[X_1]$ rewrites

$$\sum_{\ell=0}^{s} a_{2\ell} = \sum_{\ell=0}^{s} (p_{2\ell} + p_{2\ell+1}) = \sum_{\ell=0}^{2s+1} p_\ell = 1,$$

and the condition $[V_1]$ becomes

$$\sum_{\ell=1}^{s} a_{2\ell-1} = \sum_{\ell=1}^{s} (p_{2\ell} + p_{2\ell-1}) = \sum_{\ell=0}^{2s} p_\ell = 1.$$

We recall that $[X_2] - [V_2]$ yields the condition

$$-2\sum_{j=1}^{2s} (-1)^j p_j^2 = 0.$$

Order 3. First, it can be verified that the conditions $[X_3],\ [V_{3a}],\ [V_{3b}]$ are equivalent to the conditions $([X_3]-[V_{3b}])/6,\ [X_3]/6-[V_{3a}]/3+[V_{3b}]/6,\ [X_3]/6+2[V_{3a}]/3+[V_{3b}]/6$. To express in a simple way these last quantities, we now introduce $B_{3a} = \sum_{j=0}^{2s} p_j^3$ and

$$B_{3b} = \sum_{j=1}^{2s} (-1)^j p_j^2 \sum_{k=1}^{j^*} p_k,\ j^* = j-1, \text{ if } j \text{ is even},\ j^* = j, \text{ if } j \text{ is odd},$$

which can be recast in $B_{3b} = \sum_{j=1}^{s} (p_{2j}^2 - p_{2j-1}^2) \sum_{k=1}^{2j-1} p_k$. Then, we check (see the proof in the Appendix) that $([X_3] - [V_{3b}])/6$, $[X_3]/6 - [V_{3a}]/3 + [V_{3b}]/6$ and $[X_3]/6 + 2[V_{3a}]/3 + [V_{3b}]/6$ can be recast as

$$2B_{3b} + B_{3a} - \sum_{j=1}^{2s} p_j^2 (-1)^j \sum_{k=1}^{2s} p_k = 0, \tag{5.11}$$

$$B_{3b} = 0, \tag{5.12}$$

$$\left(\sum_{j=1}^{2s} p_j \right)^3 - 2B_{3b} - B_{3a} = 1. \tag{5.13}$$

Using the former conditions derived for order ≤ 2 (*i.e.* $\sum_{j=0}^{2s} (-1)^j p_j^2 = 0$ and $\sum_{j=0}^{2s} p_j = 1$), we obtain that these last equations finally reduce to $B_{3a} = 0$ and $B_{3b} = 0$.

Order 4. For the fourth order conditions $[X_{4a}], [X_{4b}], [V_{4a}], [V_{4b}], [V_{4c}]$, we introduce the notations

$$B_1 = \sum_{j=1}^{2s} p_j, \quad B_2 = \sum_{j=1}^{2s} (-1)^j p_j^2, \quad B_{4a} = \sum_{j=1}^{2s} (-1)^j p_j^4, \quad B_{4b} = \sum_{j=1}^{s} (p_{2j}^3 + p_{2j-1}^3) \sum_{k=1}^{2j-1} p_k,$$
$$B_{4c} = \sum_{j=1}^{s} (p_{2j}^2 - p_{2j-1}^2) \left(\sum_{k=1}^{j-1} p_{2k} \sum_{\ell=1}^{2k-1} p_\ell + \sum_{k=1}^{j} p_{2k-1} \sum_{\ell=1}^{2k-1} p_\ell \right),$$

and

$$M_1 = B_{4c}, \; M_2 = B_{4b}, \; M_3 = B_{4a}, \; M_4 = B_{3b} B_1,$$
$$M_5 = B_{3a} B_1, \; M_6 = B_2^2, \; M_7 = B_2 B_1^2, \; M_8 = B_1^4.$$

These notations enables to rewrite the fourth order conditions as follows (see the proof in the Appendix)

$$[X_{4a}] : 36M_1 + 12M_2 - 6M_3 - 12M_4 - 4M_5 + 9M_6 + M_8 = 1, \tag{5.14}$$
$$[X_{4b}] : 48M_1 + 24M_2 - 6M_3 - 24M_4 - 16M_5 + 15M_6 + 6M_7 + M_8 = 1, \tag{5.15}$$
$$[V_{4a}] : -12M_1 - 4M_2 + 2M_3 - 3M_6 + M_8 = 1, \tag{5.16}$$
$$[V_{4b}] : -16M_1 - 8M_2 + 2M_3 - 5M_6 + 2M_7 + M_8 = 1, \tag{5.17}$$
$$[V_{4c}] : \; -48M_1 - 24M_2 + 6M_3 + 24M_4 + 8M_5 - 9M_6 - 6M_7 + M_8 = 1. \tag{5.18}$$

Using the lower order conditions, we get $M_4 = M_5 = M_6 = M_7 = 0$ and $M_8 = 1$. Reduced expressions can then be obtained since $[V_{4a}]$, $[V_{4b}]$ and $[V_{4c}]$ produce the same condition as $[X_{4b}]$. We then deduce the following equations

$$B_{4a} - 2B_{4b} - 6B_{4c} = 0, \; B_{4a} - 4B_{4b} - 8B_{4c} = 0,$$

which can be written as

$$B_{4a} - 2B_{4b} - 6B_{4c} = 0, \; B_{4b} + B_{4c} = 0.$$

It then follows

$$B_{4b} = -B_{4a}/4, \; B_{4c} = B_{4a}/4.$$

Using these calculations, we verify that the conditions to get the order 4 are given by the equations (3.4)-(3.7) or Theorem 3.10.

6 Appendix

In the sequel, the passage from the coefficients a_{2j} to p_j needs some notations to deal with odd and even terms which make easier the computations. For example, we have

$$\sum_{j=0}^{s} a_{2j-1} \sum_{k=0}^{j-1} a_{2k} = \sum_{j=0}^{s} (p_{2j} + p_{2j-1}) \sum_{k=0}^{j-1} (p_{2k} + p_{2k+1}) = \sum_{j=0}^{2s} p_j \tilde{A}_j,$$

with $A_j = \sum_{k=0}^{j} p_k$ and

$$\tilde{A}_j = \begin{cases} A_j & \text{if} \quad j \text{ odd}, \\ A_{j-1} & \text{if} \quad j \text{ even}. \end{cases}$$

Introducing the notation $j^\star$ such that $j^\star = j$ if j is odd and $j^\star = j-1$ if j is even, we then get $\tilde{A}_j = A_{j^\star}$ and

$$\begin{aligned}\sum_{j=0}^{s} a_{2j-1} \sum_{k=0}^{j-1} a_{2k} &= \sum_{j=0}^{2s} p_j \tilde{A}_j = \sum_{j=0}^{2s} p_j A_{j^\star} = \sum_{j=0}^{2s} p_j \sum_{k=0}^{j^\star} p_k \\ &= \sum_{j=0}^{2s} p_j \left(\sum_{k<j} p_k + p_j \sin^2(j\pi/2) \right) = \sum_{j=0}^{2s} p_j \sum_{k<j} p_k + \sum_{j=0}^{2s} p_j^2 \sin^2(j\pi/2).\end{aligned}$$

The notation $j^{\star\star}$ can also be introduced, such that $j^{\star\star} = j-1$ if j is odd and $j^{\star\star} = j$ if j is even and we have

$$\begin{aligned}\sum_{j=0}^{s} a_{2j-1} \sum_{k=0}^{j} a_{2k-1} &= \sum_{j=0}^{s} (p_{2j} + p_{2j-1}) \sum_{k=0}^{j} (p_{2k-1} + p_{2k}) \\ &= \sum_{j=0}^{2s} p_j \sum_{k=0}^{j^{\star\star}} p_k = \sum_{j=0}^{2s} p_j \sum_{k<j} p_k + \sum_{j=0}^{2s} p_j^2 \cos^2(j\pi/2).\end{aligned}$$

Let us remark that another definition of the previous notations " $\star$ " is $j^\star = 2\lfloor (j-1)/2 \rfloor + 1$, $j^{\star\star} = 2\lfloor j/2 \rfloor$.

6.1 Proof of the relations for order 3

This subsection is devoted to the proofs of the fact that conditions $([X_3] - [V_{3b}])/6$, $[X_3]/6 - [V_{3a}]/3 + [V_{3b}]/6$ and $[X_3]/6 + 2[V_{3a}]/3 + [V_{3b}]/6$ can be recast as (5.11), (5.12) and (5.13).

Proof. The strategy is to express all the quantities $[X_3], [V_{3a}], [V_{3b}]$ as functions of a basis family and then to identify. This can be extended to the fourth order case in the next part. First, the condition $[X_3]/6$ is equivalent to

$$\begin{aligned}1/6 &= \sum_{\ell=0}^{s} (p_{2\ell} + p_{2\ell+1}) \sum_{k=1}^{\ell} (p_{2k} + p_{2k-1}) \sum_{j=1}^{k-1} (p_{2j} + p_{2j+1}), \\ &= \sum_{\ell=0}^{2s} p_\ell \sum_{k=1}^{\ell^{\star\star}} p_k \sum_{j=1}^{k^\star} p_j = \sum_{\ell=0}^{2s} p_\ell \sum_{k=1}^{\ell^{\star\star}} q_k,\end{aligned}$$

with $q_k = p_k \sum_{j=1}^{k^\star} p_j = p_k \sum_{j<k} p_j + p_k^2 \sin^2(k\pi/2)$. Hence we get

$$
\begin{aligned}
1/6 &= \sum_{k<\ell} p_\ell q_k + \sum_{\ell=0}^{s} p_\ell q_\ell \cos^2(\ell\pi/2),\\
&= \sum_{j<k<\ell} p_j p_k p_\ell + \sum_{k<\ell} p_\ell p_k^2 \sin^2(k\pi/2) + \sum_{j<\ell} p_l^2 p_j \cos^2(\ell\pi/2) + \sum_{\ell} p_\ell^3 \sin^2(\ell\pi/2)\cos^2(\ell\pi/2),\\
&= \sum_{j<k<\ell} p_j p_k p_\ell + \sum_{j<k} p_j^2 p_k \sin^2(j\pi/2) + \sum_{j<k} p_j p_k^2 \cos^2(k\pi/2).
\end{aligned}
$$

Second, the condition $[V_{3a}]/3$ can be recast into

$$
\begin{aligned}
1/3 &= \sum_{\ell=0}^{s} (p_{2\ell} + p_{2\ell-1}) \sum_{k=0}^{\ell-1} (p_{2k} + p_{2k+1}) \sum_{k=0}^{\ell-1} (p_{2k} + p_{2k+1}),\\
&= \sum_{\ell=0}^{2s} p_\ell \sum_{k=0}^{\ell^\star} p_k \sum_{j=0}^{\ell^\star} p_j = \sum_{\ell=0}^{2s} p_\ell \sum_{k=0}^{\ell^\star} q_k
\end{aligned}
$$

with $q_k = p_k \sum_{j=0}^{\ell^\star} p_j = p_k \sum_{j<\ell} p_j + p_k p_\ell \sin^2(\ell\pi/2)$. Hence we get

$$
\begin{aligned}
1/3 &= \sum_{\ell=0}^{2s} p_\ell \sum_{k<\ell} q_k + \sum_{\ell=0}^{2s} p_\ell q_\ell \sin^2(\ell\pi/2),\\
&= \sum_{\ell=0}^{2s} p_\ell \sum_{k<\ell} (p_k \sum_{j<\ell} p_j + p_k p_\ell \sin^2(\ell\pi/2)) + \sum_{\ell=0}^{2s} p_\ell q_\ell \sin^2(\ell\pi/2),\\
&= \sum_{\ell=0}^{2s} [p_\ell (\sum_{k<\ell} p_k)^2 + \sum_{k<\ell} p_k p_\ell^2 \sin^2(\ell\pi/2) + \sum_{j<\ell} p_\ell^2 p_j \sin^2(\ell\pi/2) + p_\ell^3 \sin^2(\ell\pi/2)],\\
&= \sum_{j>k} p_j p_k^2 + 2 \sum_{j<k<\ell} p_j p_k p_\ell + 2 \sum_{j<k} p_j p_k^2 \sin^2(k\pi/2) + \sum_{j} p_j^3 \sin^2(j\pi/2),\\
&= 2 \sum_{j<k<\ell} p_j p_k p_\ell + \sum_{j<k} p_j^2 p_k + 2 \sum_{j<k} p_j p_k^2 \sin^2(k\pi/2) + \sum_{j} p_j^3 \sin^2(j\pi/2).
\end{aligned}
$$

Finally, the condition $[V_{3b}]/6$ rewrites

$$
\begin{aligned}
1/6 &= \sum_{\ell=0}^{s} (p_{2\ell} + p_{2\ell-1}) \sum_{k=0}^{\ell-1} (p_{2k} + p_{2k+1}) \sum_{j=1}^{k} (p_{2j} + p_{2j-1}),\\
&= \sum_{\ell=0}^{2s} p_\ell \sum_{k=1}^{\ell^\star} p_k \sum_{j=1}^{k^{\star\star}} p_j = \sum_{\ell=0}^{2s} p_\ell \sum_{k=1}^{\ell^\star} q_k
\end{aligned}
$$

with $q_k = p_k \sum_{j=1}^{k^{\star\star}} p_j = p_k \sum_{j<k} p_j + p_k^2 \cos^2(j\pi/2)$. Hence, we get

$$
\begin{aligned}
1/6 &= \sum_{j<k<\ell} p_\ell p_k p_j + \sum_{k<\ell} p_\ell p_k^2 \cos^2(k\pi/2) + \sum_{j<\ell} p_\ell^2 p_j \sin^2(\ell\pi/2) + \sum_{\ell} p_\ell^3 \sin^2(\ell\pi/2)\cos^2(\ell\pi/2),\\
&= \sum_{j<k<\ell} p_j p_k p_\ell + \sum_{k<j} p_j p_k^2 \cos^2(k\pi/2) + \sum_{j<k} p_j p_k^2 \sin^2(k\pi/2).
\end{aligned}
$$

To summarize, we have

$$
\begin{aligned}
&[X_3]/6 \Longleftrightarrow 1/6 = \sum_{j<k<\ell} p_j p_k p_\ell + \sum_{j<k} p_j^2 p_k \sin^2(j\pi/2) + \sum_{j<k} p_j p_k^2 \cos^2(k\pi/2),\\
&[V_{3a}]/3 \Longleftrightarrow 1/3 = 2\sum_{j<k<\ell} p_j p_k p_\ell + \sum_{j<k} p_j^2 p_k + 2\sum_{j<k} p_j p_k^2 \sin^2(k\pi/2) + \sum_{j} p_j^3 \sin^2(j\pi/2),\\
&[V_{3b}]/6 \Longleftrightarrow 1/6 = \sum_{j<k<\ell} p_j p_k p_\ell + \sum_{j<k} p_j p_k^2 \sin^2(k\pi/2) + \sum_{j<k} p_j^2 p_k \cos^2(j\pi/2).
\end{aligned}
$$

Thus, using $(\cos^2(j\pi/2) - \sin^2(j\pi/2)) = (-1)^j$, $([V_{3b}] - [X_3])/6$ can be rewritten as

$$
0 = -\sum_{j<k} p_j p_k^2 (-1)^k + \sum_{j<k} p_j^2 p_k (-1)^j. \tag{6.1}
$$

The expression $([X_3] - 2[V_{3a}] + [V_{3b}])/6$ can be reformulated as

$$
0 = \sum_{j<k} p_j p_k^2 (-1)^k - \sum_{j} p_j^3 \sin^2(j\pi/2). \tag{6.2}
$$

And finally, $([X_3] + 4[V_{3a}] + [V_{3b}])/6$ is also

$$
1 = ([X_3] - 2[V_{3a}] + [V_{3b}])/6 + [V_{3a}],
$$

so that we get

$$
\begin{aligned}
1 &= \sum_{j<k} p_j p_k^2 (-1)^k - \sum_{j} p_j^3 \sin^2(j\pi/2)\\
&\quad + 6\sum_{j<k<\ell} p_j p_k p_\ell + 6\sum_{j<k} p_j p_k^2 \sin^2(k\pi/2) + 3\sum_{j<k} p_j^2 p_k + 3\sum_{j} p_j^3 \sin^2(j\pi/2),\\
&= 6\sum_{j<k<\ell} p_j p_k p_\ell + \sum_{j<k} p_j p_k^2 (3 - 2(-1)^k) + 3\sum_{j<k} p_j^2 p_k + 2\sum_{j} p_j^3 \sin^2(j\pi/2) \qquad (6.3)
\end{aligned}
$$

On the other side, B_{3b} is

$$
B_{3b} = \sum_{j=1}^{2s} (-1)^j p_j^2 \sum_{k=1}^{j^\star} p_k = \sum_{j<k} p_j p_k^2 (-1)^k - \sum_{j} p_j^3 \sin^2(j\pi/2),
$$

from which we rewrite the condition $([X_3] - 2[V_{3a}] + [V_{3b}])/6$ given by (6.2) into $B_{3b} = 0$.

Moreover, (5.11) can be recast into

$$\begin{aligned}
0 &= 2\sum_{j<k}(-1)^j p_j^2 p_k + 2\sum_j (-1)^j p_j^3 \sin^2(j\pi/2) + \sum_j p_j^3 - \sum_{j=1}^{2s} p_j^2(-1)^j \sum_{k=1}^{2s} p_k,\\
&= 2\sum_{j<k}(-1)^j p_j^2 p_k - \sum_{j<k} p_j^2(-1)^j p_k - \sum_{j>k} p_j^2(-1)^j p_k,\\
&= \sum_{j<k}(-1)^j p_j^2 p_k - \sum_{j<k} p_j p_k^2(-1)^k.
\end{aligned}$$

which is exactly the condition $([X_3]-[V_{3b}])/6$ given by (6.1).
We also have

$$\left(\sum_{j=0}^{2s} p_j\right)^3 = 6\sum_{j<k<\ell} p_j p_k p_\ell + 3\sum_{j<k} p_j p_k^2 + 3\sum_{j>k} p_j p_k^2 + \sum_j p_j^3.$$

Hence (5.13) becomes

$$\begin{aligned}
1 = \left(\sum_{j=1}^{2s} p_j\right)^3 &- 2B_{3b} - B_{3a},\\
&= 6\sum_{j<k<\ell} p_j p_k p_\ell + 3\sum_{j<k} p_j p_k^2 + 3\sum_{j>k} p_j p_k^2 + \sum_j p_j^3\\
&\quad - 2\sum_{j<k} p_j p_k^2(-1)^k + 2\sum_j p_j^3 \sin^2(j\pi/2) - \sum_j p_j^3,\\
&= 6\sum_{j<k<\ell} p_j p_k p_\ell + \sum_{j<k} p_j p_k^2(3-2(-1)^k) + 3\sum_{j<k} p_j^2 p_k + 2\sum_j p_j^3 \sin^2(j\pi/2),
\end{aligned}$$

which is exactly the condition $([X_3]+4[V_{3a}]+[V_{3b}])/6$ given by (6.3). ■

6.2 Proof of the relations for order 4

In this subsection, we prove that the fourth order conditions $[X_{4a}]$, $[X_{4b}]$, $[V_{4a}]$, $[V_{4b}]$ and $[V_{4c}]$ rewrite as (5.14), (5.15), (5.16), (5.17) and (5.18)

Proof. As in the previous proof, we express all the quantities $M_i, i = 1\dots,8$ as a function of a basis family. The same is performed for the conditions $[X_{4a}]$, $[X_{4b}]$, $[V_{4a}]$, $[V_{4b}]$, and $[V_{4c}]$ which then enables to find the new expression of the order conditions as a function of $M_i, i = 1,\dots,8$.
First, for simplifying the expressions, we skip the sum over ordered indices, *i.e.* instead

of writing

$$M_8 = \sum_{j<k<\ell<m} 24 p_j p_k p_\ell p_m + \sum_{j<k<\ell} 12 p_j p_k p_\ell^2 + \sum_{j<k<\ell} 12 p_j p_k^2 p_\ell + \sum_{j<k<\ell} 12 p_j^2 p_k p_\ell + \sum_{j<k} 6 p_j^2 p_k^2 + \sum_{j<k} 4 p_j^3 p_k + \sum_{j<k} 4 p_j p_k^3 + \sum_j p_j^4,$$

we just write

$$M_8 = 24 p_j p_k p_\ell p_m + 12 p_j p_k p_\ell^2 + 12 p_j p_k^2 p_\ell + 12 p_j^2 p_k p_\ell + 6 p_j^2 p_k^2 + 4 p_j^3 p_k + 4 p_j p_k^3 + p_j^4.$$

Moreover, we adopt the notation $p_j^{(k)}$ for $\sum_j (-1)^j p_j^k$.
We next calculate

$$M_7 = 2 p_j p_k p_\ell^{(2)} + 2 p_j p_k^{(2)} p_\ell + 2 p_j^{(2)} p_k p_\ell + 2 p_j p_k^{(3)} + 2 p_j^{(3)} p_k + p_j^2 p_k^{(2)} + p_j^{(2)} p_k^2 + p_j^{(4)}$$

$$M_6 = 2 p_j^{(2)} p_k^{(2)} + p_j^4 \quad \text{and} \quad M_5 = p_j p_k^3 + p_j^3 p_k + p_j^4.$$

$$M_4 = 2 p_j p_k p_\ell^{(2)} + p_j p_k^{(2)} p_\ell + p_j^2 p_k^{(2)} + \tfrac{1}{2} p_j^3 p_k - \tfrac{1}{2} p_j^{(3)} p_k + \tfrac{1}{2} p_j p_k^3 + \tfrac{1}{2} p_j p_k^{(3)} + \tfrac{1}{2} p_j^4 - \tfrac{1}{2} p_j^{(4)},$$

$$M_3 = p_j^{(4)} \quad \text{and} \quad M_2 = p_j p_k^3 + \tfrac{1}{2} p_j^4 - \tfrac{1}{2} p_j^{(4)}, \quad \text{and}$$

$$M_1 = p_j p_k p_\ell^{(2)} - \tfrac{1}{2} p_j p_k^3 + \tfrac{1}{2} p_j p_k^{(3)} + \tfrac{1}{2} p_j^2 p_k^{(2)} - \tfrac{1}{2} p_j^{(2)} p_k^{(2)} - \tfrac{1}{2} p_j^4 + \tfrac{1}{2} p_j^{(4)}.$$

On the other side, we express in the following the conditions $[X_{4a}]$, $[X_{4b}]$, $[V_{4a}]$, $[V_{4b}]$ and $[V_{4c}]$ in the same basis.

Calculation of $[X_{4a}]/12$. This relation can be written

$$\begin{aligned}
\frac{1}{12} = \sum_{j=0}^{s} a_{2j} \sum_{k=1}^{j} a_{2k-1} \sum_{\ell=0}^{k-1} a_{2\ell} \sum_{m=1}^{k-1} a_{2m} &= \sum_{j=0}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \sum_{\ell=0}^{k^\star} p_\ell \sum_{m=1}^{k^\star} p_m, \\
&= \sum_{j=0}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \sum_{\ell=0}^{k^\star} p_\ell \sum_{m<k} p_m + \sum_{j=0}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \sum_{\ell=0}^{k^\star} p_\ell p_k \sin^2(k\pi/2), \\
&= \sum_{j=0}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \left[\sum_{\ell<k} \sum_{m<k} p_\ell p_m + \sum_{m<k} p_k p_m \sin^2(k\pi/2) \right] \\
&\quad + \sum_{j=0}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \left[\sum_{\ell<k} p_\ell p_k \sin^2(k\pi/2) + p_k^2 \sin^2(k\pi/2) \right], \\
&= 2 p_j p_k p_\ell p_m + p_j^2 p_k p_\ell + p_j p_k^2 p_\ell + p_j p_k p_\ell^2 - p_j p_k^{(2)} p_\ell + p_j p_k p_\ell^{(2)} \\
&\quad + p_j^2 p_k^2/2 + p_j^2 p_k^{(2)}/2 + p_j^3 p_k/2 - p_j^{(3)} p_k/2.
\end{aligned}$$

Calculation of $[X_{4b}]/24$**.** We have

$$\frac{1}{24}=\sum_{\ell=0}^{s}a_{2\ell}\sum_{q=1}^{\ell}a_{2q-1}\sum_{p=0}^{q-1}a_{2p}\sum_{r=1}^{p}a_{2r-1},$$

$$=\sum_{j=0}^{2s}\sum_{k=0}^{j^{**}}\sum_{\ell=0}^{k^{*}}\sum_{m=0}^{\ell^{**}}p_jp_kp_\ell p_m,=\sum_{j=0}^{2s}\sum_{k=0}^{j^{**}}\sum_{\ell=0}^{k^{*}}\sum_{m=0}^{\ell-1}p_jp_kp_\ell p_m+\sum_{j=0}^{2s}\sum_{k=0}^{j^{**}}\sum_{\ell=0}^{k^{*}}p_jp_kp_\ell^2\cos^2(\ell\pi/2),$$

$$=\sum_{j=0}^{2s}\sum_{k=0}^{j^{**}}\sum_{\ell=0}^{k-1}\sum_{m=0}^{\ell-1}p_jp_kp_\ell p_m+\sum_{j=0}^{2s}\sum_{k=0}^{j^{**}}\sum_{m=0}^{k-1}p_jp_k^2\sin^2(k\pi/2)p_m+\sum_{j=0}^{2s}\sum_{k=0}^{j^{**}}\sum_{\ell=0}^{k-1}p_jp_kp_\ell^2\cos^2(\ell\pi/2),$$

$$=p_jp_kp_\ell p_m+(p_j^2p_kp_\ell+p_jp_k^2p_\ell+p_jp_kp_\ell^2+p_j^{(2)}p_kp_\ell-p_jp_k^{(2)}p_\ell+p_jp_kp_\ell^{(2)})/2$$
$$+p_j^2p_k^2/4+p_j^{(2)}p_k^2/4+p_j^2p_k^{(2)}/4+p_j^{(2)}p_k^{(2)}/4.$$

Calculation of $[V_{4a}]/4$**.** This relation can be written

$$\frac{1}{4}=\sum_{j=1}^{s}a_{2j-1}\left(\sum_{k=0}^{j-1}a_{2k}\right)^3=\sum_{j=0}^{2s}p_j\sum_{k=0}^{j^\star}p_k\sum_{\ell=0}^{j^\star}p_\ell\sum_{m=0}^{j^\star}p_m,$$

$$=\sum_{j=0}^{2s}p_j\left[\sum_{k<j}p_k\sum_{\ell<j}p_\ell\sum_{m<j}p_m+3p_j\sin^2(j\pi/2)\sum_{k<j}p_k\sum_{\ell<j}p_\ell+3p_j^2\sin^2(j\pi/2)\sum_{k<j}p_k+p_j^3\sin^2(j\pi/2)\right],$$

$$=\sum_{j=0}^{2s}p_j\left[6\sum_{m<\ell<k<j}p_kp_\ell p_m+2\sum_{k<\ell<j}p_\ell p_k^2+2\sum_{m<k<j}p_mp_k^2+\sum_{k<\ell<j}p_\ell^2p_k+\sum_{\ell<k<j}p_\ell^2p_k\right]$$

$$+3\sum_{j=0}^{2s}p_j^2\sin^2(j\pi/2)\left[2\sum_{\ell<k<j}p_kp_\ell+\sum_{k<j}p_k^2\right]+3\sum_{j}p_j^3\sin^2(j\pi/2)\sum_{m<j}p_m+\sum_{j=0}^{2s}p_j^4\sin^2(j\pi/2),$$

$$=6p_jp_kp_\ell p_m+3p_j^2p_kp_\ell+3p_jp_k^2p_\ell+3p_jp_kp_\ell^2-3p_jp_kp_\ell^{(2)}+\frac{3}{2}p_j^2(p_k^2-p_k^{(2)})+p_j^3p_k+\frac{3}{2}p_j(p_k^3-p_k^{(3)})+\frac{1}{2}(p_j^4-p_j^{(4)}).$$

Calculation of $[V_{4b}]/8$**.**

$$\frac{1}{8}=\sum_{j=1}^{s}a_{2j-1}\sum_{k=1}^{j-1}a_{2k-1}\sum_{\ell=k}^{j-1}a_{2\ell}\sum_{m=0}^{j-1}a_{2m},$$

$$=\sum_{j=1}^{2s}p_j\sum_{k=1}^{j^{\star\star}}p_k\left[\left(\sum_{\ell=0}^{j^\star}p_\ell\right)^2-\sum_{\ell=0}^{k^\star}p_\ell\sum_{m=0}^{j^\star}p_m\right]=\mathcal{A}-\mathcal{B},$$

with $\mathcal{A} = \sum_{j=1}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \left(\sum_{\ell=0}^{j^\star} p_\ell \right)^2$ and $\mathcal{B} = \sum_{j=1}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \sum_{\ell=0}^{k^\star} p_\ell \sum_{m=0}^{j^\star} p_m$. Let us first evaluate $\mathcal{A}$:

$$\mathcal{A} = \sum_{j=1}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \left(\sum_{\ell<j} p_\ell + p_j \sin^2(j\pi/2) \right) \left(\sum_{m<j} p_m + p_j \sin^2(j\pi/2) \right),$$

$$= \sum_{j=1}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \left(\sum_{\ell<j} p_\ell \sum_{m<j} p_m + 2p_j \sin^2(j\pi/2) \sum_{\ell<j} p_\ell + p_j^2 \sin^2(j\pi/2) \right),$$

$$= 2\sum_{j=1}^{2s} p_j \left[\sum_{k<j} p_k + p_j \cos^2(j\pi/2) \right] \sum_{m<\ell<j} p_\ell p_m + \sum_{j=1}^{2s} p_j \left[\sum_{k<j} p_k + p_j \cos^2(j\pi/2) \right] \sum_{\ell<j} p_\ell^2$$
$$+ 2\sum_{j=1}^{2s} p_j^2 \sin^2(j\pi/2) \sum_{k<j} p_k \sum_{\ell<j} p_\ell + \sum_{j=1}^{2s} p_j^3 \sin^2(j\pi/2) \sum_{k<j} p_k,$$

and hence

$$\mathcal{A} = 6p_j p_k p_\ell p_m + 2\sum_{j=1}^{2s} p_j \left(\sum_{k<\ell<j} p_\ell p_k^2 + \sum_{m<k<j} p_m p_k^2 \right) + p_j p_k (p_\ell^2 + p_\ell^{(2)})$$
$$+ \sum_{j=1}^{2s} p_j \left(\sum_{k<\ell<j} p_k p_\ell^2 + \sum_{\ell<k<j} p_k p_\ell^2 + \sum_{k<j} p_k^3 \right) + p_j^2 (p_k^2 + p_k^{(2)})/2$$
$$+ 2p_j p_k (p_\ell^2 - p_\ell^{(2)}) + p_j^2 (p_k^2 - p_k^{(2)}) + p_j (p_k^3 - p_k^{(3)})/2,$$
$$= 6p_j p_k p_\ell p_m + 3p_j^2 p_k p_\ell + 3p_j p_k^2 p_\ell + 3p_j p_k p_\ell^2 - p_j p_k p_\ell^{(2)} + \frac{3}{2} p_j^2 p_k^2 - \frac{1}{2} p_j^2 p_k^{(2)} + p_j^3 p_k + p_j (p_k^3 - p_k^{(3)})/2.$$

Let then calculate $\mathcal{B}$

$$\mathcal{B} = \sum_{j=1}^{2s} p_j \sum_{k=1}^{j^{\star\star}} p_k \sum_{\ell=0}^{k^\star} p_\ell \sum_{m=0}^{j^\star} p_m,$$
$$= \sum_{j=1}^{2s} p_j \left(\sum_{k<j} p_k + p_j \cos^2(j\pi/2) \right) \left(\sum_{\ell<k} p_\ell + p_k \sin^2(k\pi/2) \right) \left(\sum_{m<j} p_m + p_j \sin^2(j\pi/2) \right),$$

whence

$$\mathcal{B} = \sum_j p_j \sum_{\ell<k<j} p_\ell p_k (\sum_{m<j} p_m + p_j \sin^2(j\pi/2)) + \sum_j p_j^2 \cos^2(j\pi/2) \sum_{\ell<j} p_\ell (\sum_{m<j} p_m + p_j \sin^2(j\pi/2))$$
$$+ \sum_j p_j \sum_{k<j} p_k^2 \sin^2(k\pi/2)(\sum_{m<j} p_m + p_j \sin^2(j\pi/2)).$$

This shows that

$$\begin{aligned}\mathcal{B} = 3p_jp_kp_\ell p_m + \sum_{\ell<k<j} p_jp_kp_\ell^2 + \sum_{\ell<k<j} p_jp_k^2p_\ell + \sum_{\ell<k<j} p_\ell p_kp_j^2\sin^2(j\pi/2) \\ + \sum_j p_j^2\cos^2(j\pi/2)\sum_{\ell<j}p_\ell\sum_{m<j}p_m \\ + \sum_{m<k<j} p_jp_k^2\sin^2(k\pi/2)p_m + \sum_{k<m<j} p_jp_k^2\sin^2(k\pi/2)p_m + \sum_{k<j}p_jp_k^3\sin^2(k\pi/2) \\ + \sum_{k<j}p_j^2\sin^2(j\pi/2)p_k^2\sin^2(k\pi/2),\end{aligned}$$

$$\begin{aligned}&= 3p_jp_kp_\ell p_m + p_j^2p_kp_\ell + p_jp_k^2p_\ell + p_jp_k(p_\ell^2 - p_\ell^{(2)})/2 + 2p_jp_k(p_\ell^2+p_\ell^{(2)})/2 + p_j^2(p_k^2+p_k^{(2)})/2 \\ &+ p_j(p_k^2-p_k^{(2)})/2\ p_\ell + (p_j^2-p_j^{(2)})/2\ p_kp_\ell + (p_j^3-p_j^{(3)})/2\ p_k + (p_j^2-p_j^{(2)})(p_k^2-p_k^{(2)})/4, \\ &= 3p_jp_kp_\ell p_m + \frac{3}{2}p_j^2p_kp_\ell + \frac{3}{2}p_jp_k^2p_\ell + \frac{3}{2}p_jp_kp_\ell^2 - \frac{1}{2}p_j^{(2)}p_kp_\ell - \frac{1}{2}p_jp_k^{(2)}p_\ell + \frac{1}{2}p_jp_kp_\ell^{(2)} + \frac{3}{4}p_j^2p_k^2 \\ &\qquad + \frac{1}{4}p_j^2p_k^{(2)} - \frac{1}{4}p_j^{(2)}p_k^2 + \frac{1}{4}p_j^{(2)}p_k^{(2)} + (p_j^3-p_j^{(3)})/2\ p_k.\end{aligned}$$

We then obtain the following expression for $[V_{4b}]/8$

$$\begin{aligned}\frac{1}{8} &= 3p_jp_kp_\ell p_m + \frac{3}{2}(p_j^2p_kp_\ell + p_jp_k^2p_\ell + p_jp_kp_\ell^2) + \frac{1}{2}(p_j^{(2)}p_kp_\ell + p_jp_k^{(2)}p_\ell - 3p_jp_kp_\ell^{(2)}) \\ &+ \frac{3}{4}p_j^2p_k^2 - \frac{3}{4}p_j^2p_k^{(2)} + \frac{1}{4}p_j^{(2)}p_k^2 - \frac{1}{4}p_j^{(2)}p_k^{(2)} + \frac{1}{2}p_j(p_k^3 - p_k^{(3)}) + \frac{1}{2}(p_j^3+p_j^{(3)})p_k\end{aligned}$$

Calculation of $[V_{4c}]/24$**.**

$$\frac{1}{24} = \sum_{j=1}^{s} a_{2j-1}\sum_{k=1}^{j-1}a_{2k-1}\sum_{\ell=k}^{j-1}a_{2\ell}\sum_{m=0}^{k-1}a_{2m} = \mathcal{B} - B$$

with $B = \sum_{j=1}^{2s}p_j\sum_{k=1}^{j^{\star\star}}p_k\sum_{\ell=0}^{k^\star}p_\ell\sum_{m=0}^{k^\star}p_m = 1/12$ (using the first line of the computation of $[X_{4a}]/12$).

Assembling conditions (5.14), (5.15), (5.16), (5.17) and (5.18) using the new expressions of $M_i, i=1,\ldots,8$ enables to recover the order conditions $[X_{4a}]$, $[X_{4b}]$, $[V_{4a}]$, $[V_{4b}]$ and $[V_{4c}]$, which ends the proof. ■

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