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SIMPLIFIED ORDER CONDITIONS OF SOME CANONICAL DIFFERENCE SCHEMES*1)

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Abstract

The main purpose of this paper is to develop and simplify the general conditions for an s-stage explicit canonical difference scheme of q-th order, while the simplified order conditions for canonical RKN methods which are applied to a special kind of second order ordinary differential equations are also obtained here.

1. Introduction

In [5–8], explicit canonical difference schemes up to the fourth order are constructed for separable Hamiltonian systems (i.e., systems with the Hamiltonian function $H(p,q)=U(p)+V(q)$). But unfortunately, we can not find the general order conditions for this method whether sn algebraic or Lie method is used to get order conditions for some scheme of a definite stage number. In this paper, we will use P-series introduced in [4] and tree methodology used by Sanz-Serna in [2] to get the general order conditions for the explicit canonical method and then simplify these conditions to get much more independent ones.

In [12], we have already omitted some redundant order conditions for canonical RKN methods, but there are still some order conditions dependent on each other because of the canonicity of the methods. In this paper, we will drop out these order conditions and get much simpler ones.

In Section 1, we give some definitions and notations about graphs and trees; they are the basis of understanding the later derivation in Sections 2 and 3. Section 2 is about general order conditions of canonical explicit methods and their simplified form. In Section 3, we get simplified order conditions of the canonical RKN method.

1. Graphs and Trees

In this section, we only give some definitions and notations about graphs and trees which will be used in this paper. For details about graphs and trees, one can refer to [2],[4].

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1. Graphs. Let n be a positive integer. A **graph** G of **order** n is a pair $\{V, E\}$ formed by a set V with $\mathrm{Card}(V) = n$ and a set E of un-ordered pairs (v, w), with $v, w \in V, v \neq w$, which may be empty. The elements of V and E are called **vertices** and **edges** of the graph respectively. Two vertices v, w are called **adjacent** if $(v, w) \in E$.

Graphs can be represented graphically as Fig. 1 shows. In Figure 1, the black dots represent the vertices of the graph, and the lines joining the dots are the edges.

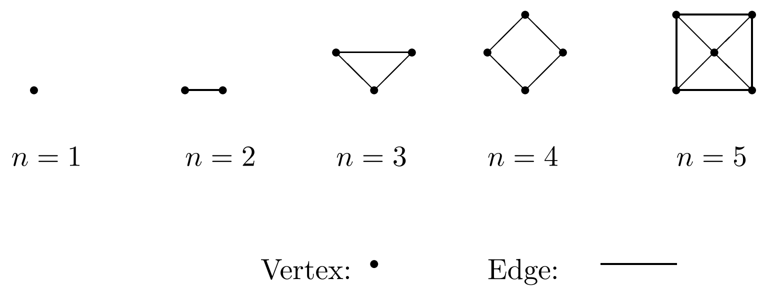

Fig. 1. Graphs

Giving the vertices of G an arbitrary set of labels, we then get a **labeled graph** $g, g \in G$. By labeling the graph G in different ways, we can get different labeled graphs. For convenience, we often use letters $i, j, k, l, \cdots$ as the labels in this paper. Notice that in the definition of the graph G, we use v and w to denote two different vertices; they are not the labels of these vertices. Fig. 2 shows a graph of order 4 and its different labelings.

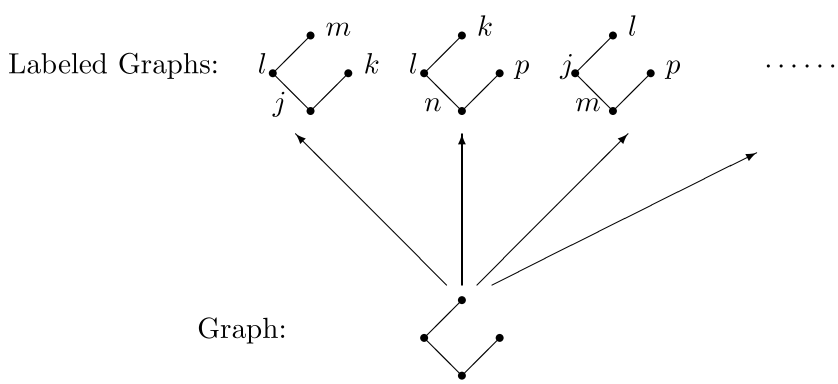

Fig. 2. Graphs and Labeled Graphs

Now we consider two kinds of special graphs: P-graphs and S-graphs.

A **P-graph** PG is a special graph which satisfies:

i) its vertices are divided into two classes: **"white"** and **"black"**;

i) the two adjacent vertices of a PG cannot be of the same class.

Fig.3 shows some examples of P-graphs:

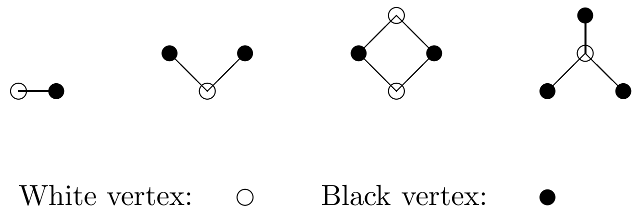

Fig. 3. P-Graphs

An **S-graph** SG is a special P-graph of which white vertices have no more than two adjacent black vertices. **Labeled P-graph** and **labeled S-graph** are defined as the labeled graph. Fig. 4 shows some examples of S-graphs:

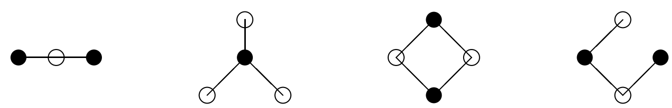

Fig. 4. S-Graphs

A **simple path** joining a pair of vertices v and $w, v \neq w$, is a sequence of pairwise distinct vertices $v = v_0, v_1, \cdots, v_m = w$, with v_i adjacent to $v_{i+1}, i = 0, 1, \cdots, m-1$.

2. Trees. (a) A **tree** t of order n is a graph G of the same order such that for any pair of distinct vertices of V there exists a unique simple path that joins them. A **rooted tree** Rt is a tree with one of its vertex regarded as the **root** of the whole tree. Giving the vertices of the tree t (resp. rooted tree Rt) an arbitrary set of labels, we get a **labeled tree** RLt (resp. rooted labeled tree RSt); we say $Lt \in t$(resp. $RLt \in Rt$). The vertices adjacent to the root are called its **sons**. The sons of the remaining vertices are defined in an obviously recursive way. Fig. 5 shows a tree and different rooted trees got from it.

In fact, once a vertex r is regarded as the root, the previous un-ordered edges in E (i.e., the pairs of vertices in E) are ordered under the **son to father projection** $T : v \longrightarrow w$, where v and w are the son and father respectively. This projection T has a single value.

(b) The definitions of a **P-tree** Pt, a **labeled P-tree** LPt, a **rooted P-tree** RPt and a **rooted labeled P-tree** $RLPt$ of the same order n are just as those of tree t, labeled tree Lt, rooted tree Rt and rooted labeled tree RLt. However, the general graph is substituted by the P-graph; so are the definitions of the **S-tree** St, **labeled S-tree** LSt, **rooted S-tree** RSt and **rooted labeled S-tree** $RLSt$.

We should point out that in this paper, we consider only S-trees with black root vertices. So when we refer to a rooted S-tree, we means that it is an S-tree with black vertex.

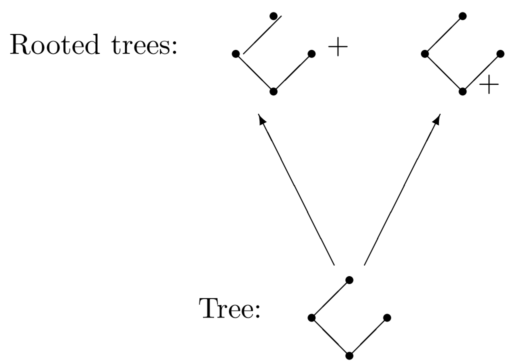

Fig. 5. Tree and rooted trees[1)]

(c) If we give the vertices of a rooted P-tree RPt such a set of labels so that the label of a father vertex is always smaller than that of its sons, we then get a **monotonically labeled rooted P-tree** $MRLPt$. We denote by $\alpha(RPt)$ the number of possible different monotonic labelings of RPt when the labels are chosen from the set $A_q = \{$ the first q letters of $i < j < k < l < \cdots\}$, where q is the order of RPt.

(d) Denote by RPt_a(resp. RPt_b) a rooted P-tree RPt that has a white(resp. black) root. The set of all rooted P-trees of order n with a meager(resp. black) root is denoted by TP_n^a(resp. TP_n^b). Denote by LPt_n^a(resp. LPt_n^b) the set of all rooted labeled P-trees of order n with a white (resp. black) root vertex, and $MLTP_n^a$(resp. $MLTP_n^b$) the set of all monotonically labeled P-trees of order n with a white (resp. black) root vertex when the labels are chosen from the set A_n.

(e) Let $RPt^1, \cdots, RPt^m$ be rooted P-trees. We denote by $RPt =_a [RPt^1, \cdots, RPt^m]$ the unique rooted P-tree that arises when the roots of $RPt^1, \cdots, RPt^m$ are all attached to a white root vertex. Similarly, denote by $_b[RPt^1, \cdots, RPt^m]$ when the root of the P-tree is black. We say $RPt^1, \cdots, RPt^m$ are **sub-trees** of RPt. We further denote by τ_a(resp. τ_b) the rooted P-trees of order 1 which has a white(resp. black) root vertex.

(f) The **density** $\gamma(Rt)$ of a rooted tree Rt is defined recursively as

$$\gamma(Rt) = \rho(Rt)\gamma(Rt^1)\cdots\gamma(Rt^m),$$

where $\rho(Rt)$ is the order of Rt and $Rt^1, \cdots, Rt^m$ are the sub-trees which arise when the root of Rt is moved from the tree. The density of rooted P-tree RPt and rooted S-tree RSt are calculated by regarding them as general rooted trees with the difference between the black and white vertices playing no role.

[1)] The vertex with "+" is the root.

2. General Order Conditions of Explicit Canonical Schemes

2.1. Order conditions of explicit canonical schemes

Consider the Hamiltonian system

$$\begin{cases} \dfrac{dp}{dt} = -H_q, \\ \dfrac{dq}{dt} = H_p, \end{cases} \tag{1}$$

where $p = [p^1, \cdots, p^n]^T$, $q = [q^1, \cdots, q^n]^T$, $H_p = \dfrac{\partial H}{\partial p} = \left[\dfrac{\partial H}{\partial p^1}, \cdots, \dfrac{\partial H}{\partial p^n}\right]^T$, $H_q = \dfrac{\partial H}{\partial q} = \left[\dfrac{\partial H}{\partial q^1}, \cdots, \dfrac{\partial H}{\partial q^n}\right]^T$. When $H = U(p) + V(q)$, we have

$$\begin{cases} \dfrac{dp}{dt} = -H_q = -\dfrac{\partial V}{\partial q} = f(q), \\ \dfrac{dq}{dt} = H_p = \dfrac{\partial U}{\partial p} = g(p). \end{cases} \tag{2}$$

It is well known that the following $(s-1)$-stage scheme

$$\begin{cases} p_i = p_{i-1} + c_i h f(q_{i-1}), \\ q_i = q_{i-1} + d_i h g(p_i), \end{cases} \quad i = 1, \cdots, s-1 \tag{3}$$

where p_0, q_0 are initial values and h is the step-size, is canonical when used to solve system (2).

Let $p = y_a, q = y_b, f = f_a, g = f_b$ and $y_{a,0} = p_0, y_{b,0} = q_0, y_{a,1} = p_{s-1}, y_{b,1} = q_{s-1}$. Then (3) is transformed into an s-stage scheme of partitioned Runge-Kutta form

$$\begin{cases} g_{1,a} = y_{a,0} = p_0, \\ g_{1,b} = y_{b,0} = q_0, \\ g_{2,a} = y_{a,0} + c_1 h f_a(q_0) = y_{a,0} + c_1 h f_a(g_{1,b}) = p_1, \\ g_{2,b} = y_{b,0} + d_1 h f_b(p_1) = y_{b,0} + d_1 h f_b(g_{2,a}) = q_1, \\ \vdots \\ g_{s,a} = y_{a,0} + h \displaystyle\sum_{j=1}^{s-1} c_j f_a(g_{j,b}) = p_{s-1}, \\ g_{s,b} = y_{b,0} + h \displaystyle\sum_{j=1}^{s-1} d_j f_b(g_{j+1,a}) = q_{s-1}. \end{cases} \tag{4}$$

(4) can be written equivalently as

$$\begin{cases} y_{a,1} = y_{a,0} + h\sum_{i=1}^{s-1} c_i f_a(g_{i,b}), \\ y_{b,1} = y_{b,0} + h\sum_{i=1}^{s-1} d_i f_b(g_{i+1,a}), \\ g_{i,a} = y_{a,0} + h\sum_{j=1}^{i-1} c_j f_a(g_{j,b}), \quad \text{for} \quad i = 1, \cdots, s, \\ g_{i,b} = y_{b,0} + h\sum_{j=1}^{i-1} d_j f_b(g_{j+1,a}), \quad \text{for} \quad i = 1, \cdots, s. \end{cases} \tag{5}$$

And (2) can be rewritten with new variables as

$$\begin{bmatrix} y_a \\ \\ y_b \end{bmatrix} = \begin{bmatrix} f_a(y_b) \\ \\ f_b(y_a) \end{bmatrix}. \tag{6}$$

Let

$$\begin{cases} a_1 = c_1, \quad a_2 = c_2, \ \cdots, \ a_{s-1} = c_{s-1}, \quad a_s = 0, \\ \\ b_1 = 0, \quad b_2 = d_1, \ \cdots, \ b_{s-1} = d_{s-2}, \quad b_s = d_{s-1} \end{cases}$$

Scheme (5) now becomes

$$\begin{cases} y_{a,1} = y_{a,0} + \sum_{i=1}^{s} a_i k_{i,a}, \\ y_{b,1} = y_{b,0} + \sum_{i=1}^{s} b_i k_{i,b}, \\ g_{i,a} = y_{a,0} + h\sum_{j=1}^{i-1} a_j f_a(g_{j,b}) = y_{a,0} + \sum_{j=1}^{i-1} a_j k_{j,a}, \quad \text{for} \quad i = 1, \cdots, s, \\ g_{i,b} = y_{b,0} + h\sum_{j=1}^{i} b_j f_b(g_{j,a}) = y_{b,0} + \sum_{j=1}^{i} b_j k_{j,b}, \quad \text{for} \quad i = 1, \cdots, s, \end{cases} \tag{7}$$

where

$$k_{i,a} = hf_a(g_{i,b}), \quad k_{i,b} = hf_b(g_{i,a}). \tag{8}$$

We now just need to study the order conditions of scheme (8) when $a_s = b_1 = 0$. Notice that $a_s = b_1 = 0$ is necessary for (8) to be canonical and is also crucial for simplifying order conditions as we will see later.

Before we use P-trees and P-series to derive the order conditions, we should define elementary differentials. The **elementary differentials** F corresponding to system

(6) are defined recursively as

$$\begin{cases} F(\tau_a)(y) = f_a(y), F(\tau_b)(y) = f_b(y), \\ F(RPt) = \dfrac{\partial^m f_{W(RPt)}(y)}{\partial y_{W(RPt^1)} \cdots \partial y_{W(RPt^m)}} (F(RPt^1)(y), \cdots, F(RPt^m)(y)), \end{cases} \tag{9}$$

where $y = (y_a, y_b)$ and $RPt =_{W(RPt)} [RPt^1, \cdots, RPt^m]$. In (9),

$$W(RPt) = \begin{cases} a, & \text{if the root of } RPt \text{ is white}, \\ b, & \text{if the root of } RPt \text{ is black}. \end{cases}$$

We see $F(RPt)$ is independent of labeling. Here, and in the remainder of this paper, in order to avoid sums and unnecessary indices, we assume that y_a and y_b in (6) are scalar quantities, and f_a, f_b scalar functions. All subsequent formulas remain valid for vectors if the derivatives are interpreted as multi-linear mappings. For details about elementary differentials, see [4].

From [4], we have the following theorem:

Theorem 1. *The derivatives of the exact solution of* (6) *satisfy*

$$\begin{cases} y_a^{(q)} = \displaystyle\sum_{RLPt \in MLTP_q^a} F(RLPt)(y_a, y_b) = \sum_{RPt \in TP_q^a} \alpha(RPt) F(RPt)(y_a, y_b), \\ y_b^{(q)} = \displaystyle\sum_{RLPt \in MLTP_q^b} F(RLPt)(y_a, y_b) = \sum_{RPt \in TP_q^b} \alpha(RPt) F(RPt)(y_a, y_b). \end{cases} \tag{10}$$

It is convenient to introduce two new "rooted" P-trees of order 0: ϕ_a and ϕ_b. Their corresponding elementary differentials are $F(\phi_a) = y_a, F(\phi_b) = y_b$. We further set

$$TP^a = \phi_a \cup TP_1^a \cup TP_2^a \cup \cdots$$

$$TP^b = \phi_b \cup TP_1^b \cup TP_2^b \cup \cdots$$

$$LTP^a = \phi_a \cup LTP_1^a \cup LTP_2^a \cup \cdots$$

$$LTP^b = \phi_b \cup LTP_1^b \cup LTP_2^b \cup \cdots$$

$$MLTP^a = \phi_a \cup MLTP_1^a \cup MLTP_2^a \cup \cdots$$

$$MLTP^b = \phi_b \cup MLTP_1^b \cup MLTP_2^b \cup \cdots.$$

Now we can give the definition of P-series:

P-series. Let $C(\phi_a), C(\phi_b), C(\tau_a), C(\tau_b), \cdots$, be real coefficients defined for all P-trees

$$C: \ TP^a \cup TP^b \longrightarrow R.$$

The series $P(C,y)=(P_a(C,y),P_b(C,y))^T$ is defined as

$$\begin{aligned}
P_a(C,y) &= \sum_{RLPt\in MLTP^a}\frac{h^{\rho(RLPt)}}{\rho(RLPt)!}C(RLPt)F(RLPt)(y)\\
&= \sum_{RPt\in TP^a}\alpha(RPt)\frac{h^{\rho(RPt)}}{\rho(RPt)!}C(RPt)F(RPt)(y),\\
P_b(C,y) &= \sum_{RLPt\in MLTP^b}\frac{h^{\rho(RLPt)}}{\rho(RLPt)!}C(RLPt)F(RLPt)(y)\\
&= \sum_{RPt\in TP^b}\alpha(RPt)\frac{h^{\rho(RPt)}}{\rho(RPt)!}C(RPt)F(RPt)(y).
\end{aligned} \tag{11}$$

Notice that C is defined on $TP^a\cup TP^b$, and for two different labelings $RLPt^1$ and $RLPt^2$ (especially, for monotonic labelings $MRLPt^1$ and $MRLPt^2$) of the same rooted P-tree RPt, we have $C(RLPt^1)=C(RLPt^2)(\text{especially}, C(MRLPt^1)=C(MRLPt^2))$.

Theorem 1 states simply that the exact solution of (6) is a P-series

$$(y_a(t_0+h),y_b(t_0+h))^T=P(Y,(y_a(t_0),y_b(t_0)))$$

with $Y(RPt)=1$ for all rooted P-trees RPt.

Theorem 2. *Let $C: TP^a\cup TP^b\longrightarrow R$, be a sequence of coefficients such that $C(\phi_a)=C(\phi_b)=1$. Then*

$$h\begin{bmatrix} f_a(P(C,(y_a,y_b)))\\ f_b(P(C,(y_a,y_b)))\end{bmatrix}=P(C',(y_a,y_b))$$

with

$$\begin{aligned}
&C'(\phi_a)=C'(\phi_b)=0,\\
&C'(\tau_a)=C'(\tau_b)=1,\\
&C'(RPt)=\rho(RPt)C(RPt^1)\cdots C(RPt^m)
\end{aligned}$$

if $RPt=_{W(RPt)}[RPt^1,\cdots,RPt^m]$.

The proof is given in [4].

Let

$$\begin{cases}
k_{i,a}=P_a(K_i,(y_{a,0},y_{b,0})),\\
k_{i,b}=P_b(K_i,(y_{a,0},y_{b,0})),\\
g_{i,a}=P_a(G_i,(y_{a,0},y_{b,0})),\\
g_{i,b}=P_b(G_i,(y_{a,0},y_{b,0})),
\end{cases}\qquad \text{for}\quad i=1,\cdots,s,$$

where $K_i(i=1,\cdots,s):TP^a\cup TP^b\longrightarrow R$ and $G_i(i=1,\cdots,s):TP^a\cup TP^b\longrightarrow R$ are two sets of P-series. From (5), we have $G_i(\phi_a)=G_i(\phi_b)=1$. Hence

$$\begin{aligned}
P(K_i,(y_{a,0},y_{b,0})) &= \begin{bmatrix} P_a(K_i,(y_{a,0},y_{b,0})) \\ P_b(K_i,(y_{a,0},y_{b,0})) \end{bmatrix} = \begin{bmatrix} k_{i,a} \\ k_{i,b} \end{bmatrix} = h\begin{bmatrix} f_a(g_{i,b}) \\ f_b(g_{i,a}) \end{bmatrix} \\
&= h\begin{bmatrix} f_a(P_b(G_i,(y_{a,0},y_{b,0}))) \\ f_b(P_a(G_i,(y_{a,0},y_{b,0}))) \end{bmatrix} = h\begin{bmatrix} f_a(P(G_i,(y_{a,0},y_{b,0}))) \\ f_b(P(G_i,(y_{a,0},y_{b,0}))) \end{bmatrix} \\
&= P(G_i',(y_{a,0},y_{b,0})).
\end{aligned}$$

Then, from Theorem 2 we have

$$K_i=G_i',\quad i=1,\cdots,s. \tag{12}$$

But from (7) we have

$$P(G_i,(y_{a,0},y_{b,0}))=\begin{bmatrix} P_a(G_i,(y_{a,0},y_{b,0})) \\ P_b(G_i,(y_{a,0},y_{b,0})) \end{bmatrix}=\begin{bmatrix} y_{a,0}+\sum_{j=1}^{i-1}a_jk_{j,a} \\ y_{b,0}+\sum_{j=1}^{i}b_jk_{j,b} \end{bmatrix}$$

$$=\begin{bmatrix} y_{a,0}+\sum_{j=1}^{i-1}a_jP_a(K_j,(y_{a,0},y_{b,0})) \\ y_{b,0}+\sum_{j=1}^{i}b_jP_b(K_j,(y_{a,0},y_{b,0})) \end{bmatrix}=\begin{bmatrix} y_{a,0}+P_a\left(\sum_{j=1}^{i-1}a_jK_j,(y_{a,0},y_{b,0})\right) \\ y_{b,0}+P_b\left(\sum_{j=1}^{i}b_jK_j,(y_{a,0},y_{b,0})\right) \end{bmatrix}$$

for $i=1,\cdots,s$. Thus

$$\begin{cases} G_i(RPt_a)=\sum_{j=1}^{i-1}a_jK_j(RPt_a), \\ G_i(RPt_b)=\sum_{j=1}^{i}b_jK_j(RPt_b) \end{cases} \tag{13}$$

for $\rho(RPt_a),\rho(RPt_b)\geq 1$ and $i=1,\cdots,s$. From (7) we also have

$$\begin{cases} y_{a,1}=y_{a,0}+\sum_{i=1}^{s}a_iP_a(K_i,(y_{a,0},y_{b,0})), \\ y_{b,1}=y_{b,0}+\sum_{i=1}^{s}b_iP_b(K_i,(y_{a,0},y_{b,0})). \end{cases} \tag{14}$$

Comparing the numerical solution got from (7) with the exact solution, we get the conditions for scheme (7) of p-th order.

Theorem 3. *The scheme* (7) *is of p-th order iff*

$$\begin{cases} \sum_{i=1}^{s} a_i K_i(RPt_a) = 1, \\ \sum_{i=1}^{s} b_i K_i(RPt_b) = 1, \end{cases} \quad \textit{for} \quad 1 \le \rho(RPt_a), \rho(RPt_b) \le p, \tag{15}$$

where $K_i (i = 1, \cdots, s)$ *are defined recursively by*

$$\begin{cases} K_i = G_i', \quad G_i(\phi_a) = G_i(\phi_b) = 1, \\ G_i(RPt_a) = \sum_{j=1}^{i-1} a_j K_j(RPt_a), \\ G_i(RPt_b) = \sum_{j=1}^{i} b_j K_j(RPt_b), \end{cases} \quad \textit{for} \quad i = 1, \cdots, s. \tag{16}$$

2.2. Simplified order conditions

We now define **elementary weight** $\Phi(RPt)$ for a rooted P-tree RPt. Choose one labeling of RPt, for convenience, say a monotonic one with labels $i < j < k < \cdots$. For simplicity, we just denote this monotonically labeled P-tree as $RLPt$. Let $RLPt =_{W(RLPt)} [RLPt^1, \cdots, RLPt^m]$. We first define $\Phi(RLPt)$ recursively as

$$\Phi(RLPt) = \begin{cases} \sum_{i=1}^{f(r)-1} a_r(\Phi(RLPt^1) \cdots \Phi(RLPt^m)), & \text{for} \quad W(RLPt) = a, \\ \sum_{i=1}^{f(r)} b_r(\Phi(RLPt^1) \cdots \Phi(RLPt^m)), & \text{for} \quad W(RLPt) = b, \end{cases} \tag{17}$$

where r is the label of the root of $RLPt$ and $f(r)$ is the label of the father of r.

When we compute the elementary weight of a rooted labeled P-tree $RLPt$ regarded as an original tree, that is, not a sub-tree of another big tree, we add an imaginary father vertex always labeled s to the root i of $RLPt$, while the roots of its sub-trees $\Phi(RLPt^1), \cdots, \Phi(RLPt^m)$ have the same father vertex which is the root of $RLPt$ with label i. If we compute the elementary weight of rooted labeled P-tree $RLPt$ regarding it as a sub-tree of another big tree, we notice that the root of $RLPt$ has a father vertex in the original tree. So a rooted P-tree has different elementary weights when it acts as an original tree and as a sub-tree.

From the form of (17), we know the elementary weights of two labeled P-trees $RPt^1, RPt^2 \in RPt$ are same and choosing monotonic labeling is unnecessary. Thus the elementary weight of an original rooted P-tree RPt can be defined as $\Phi(RPt) = \Phi(RLPt)$ for any $RLPt \in RPt$.

Theorem 4. *Order conditions in* (15) *are equivalent to*

$$\Phi(RPt) = \frac{1}{\gamma(RPt)} \quad \textit{for} \quad RPt \in TP^a \cup TP^b, \ \rho(RPt) \le p. \tag{18}$$

Proof. We just have to prove

$$\begin{cases} \Phi(RLPt_a)\gamma(RLPt_a) = \sum_{i=1}^{s} a_i K_i(RLPt_a), \\ \Phi(RLPt_b)\gamma(RLPt_b) = \sum_{i=1}^{s} b_i K_i(RLPt_b), \end{cases} \tag{19}$$

where $RLPt_a, RLPt_b$ are monotonically labeled P-trees with labels $i < j < k < l < \cdots$, $RLPt_a \in RPt_a, RLPt_b \in RPt_b$.

From (16), we have

$$\begin{cases} K_i(RLPt_a) = \rho(RLPt_a)\left(\sum_{j_1=1}^{i} b_{j_1} K_{j_1}(RPLt_b^1)\right)\cdots\left(\sum_{j_{m_1}=1}^{i} b_{j_{m_1}} K_{j_{m_1}}(RLPt_b^{m_1})\right), \\ K_i(RLPt_b) = \rho(RLPt_b)\left(\sum_{j_{m_1}=1}^{i-1} a_{j_1} K_{j_1}(RLPt_a^1)\right)\cdots\left(\sum_{j_{m_2}=1}^{i} a_{j_{m_2}} K_{j_{m_2}}(RLPt_a^{m_2})\right) \end{cases} \tag{20}$$

where

$$\begin{cases} RLPt_a =_a [RLPt_b^1, \cdots, RLPt_b^{m_1}], \\ RLPt_b =_b [RLPt_a^1, \cdots, RLPt_a^{m_2}], \end{cases} \tag{21}$$

while $j_1, \cdots, j_{m_1}$ and $j_1, \cdots, j_{m_2}$ are the labels of the roots of $RLPt_b^1, \cdots, RLPt_b^{m_1}$ and $RLPt_a^1, \cdots, RLPt_a^{m_2}$ respectively.

Thus from (17),(20) and the definition of γ, we have

$$\text{Right side of} \quad (21) \Longleftrightarrow$$

$$\begin{cases} \sum_{i=1}^{s} a_i \rho(RLPt_a)\Big(\sum_{j_1=1}^{i} b_{j_1} K_{j_1}(RLPt_b^1)\Big)\cdots\Big(\sum_{j_{m_1}=1}^{i} b_{j_{m_1}} K_{j_{m_1}}(RLPt_b^{m_1})\Big), \\ \sum_{i=1}^{s} b_i \rho(RLPt_b)\Big(\sum_{j_1=1}^{i-1} a_{j_1} K_{j_1}(RLPt_a^1)\Big)\cdots\Big(\sum_{j_{m_2}=1}^{i-1} a_{j_{m_2}} K_{j_{m_2}}(RLPt_a^{m_2})\Big), \end{cases}$$

$$\text{Left} - \text{sideof} \quad (21) \Longleftrightarrow$$

$$\begin{cases} \sum_{i=1}^{s} a_i \rho(RLPt_a)(\Phi(RLPt_b^1)\gamma(RLPt_b^1))\cdots(\Phi(RLPt_b^{m_1})\gamma(RLPt_b^{m_1})), \\ \sum_{i=1}^{s} b_i \rho(RLPt_b)(\Phi(RLPt_a^1)\gamma(RLPt_a^1))\cdots(\Phi(RLPt_a^{m_2})\gamma(RLPt_a^{m_2})). \end{cases}$$

So we have to prove

$$\begin{cases} \Phi(RLPt_b^n)\gamma(RLPt_b^n) = \sum_{j_n=1}^{i} b_{j_n} k_{j_n}(RLPt_b^n) \quad \text{for} \quad n = 1, 2, \cdots, m_1, \\ \Phi(RLPt_a^n)\gamma(RLPt_a^n) = \sum_{j_n=1}^{i-1} a_{j_n} k_{j_n}(RLPt_a^n) \quad \text{for} \quad n = 1, 2, \cdots, m_2. \end{cases}$$

Continue this process and finally we see it is enough to prove

$$\begin{cases} \Phi(\tau_a)\gamma(\tau_a) = \displaystyle\sum_{r=1}^{f(r)-1} a_r K_r(\tau_a), \\ \Phi(\tau_b)\gamma(\tau_b) = \displaystyle\sum_{r=1}^{f(r)} b_r K_r(\tau_b), \end{cases} \tag{22}$$

where r is the label of τ_a or τ_b and $f(r)$ is the label of its father. Since

$$\begin{cases} \Phi(\tau_a)\gamma(\tau_a) = \left(\displaystyle\sum_{r=1}^{f(r)-1} a_r\right) \cdot 1, \\ \Phi(\tau_b)\gamma(\tau_b) = \left(\displaystyle\sum_{r=1}^{f(r)} b_r\right) \cdot 1 \end{cases} \quad \text{and} \quad \begin{cases} K_r(\tau_a) = 1, \\ K_r(\tau_b) = 1, \end{cases}$$

we have finished the proof.

Let Pt be a P-tree of order $n \geq 2$. Let v and w be two adjacent vertices. We consider four rooted P-trees as follows. Denote by RPt^v(resp. RPt^w) the rooted P-tree obtained by regarding the vertex v(resp. w) as the root of Pt. Denote by $RPtv$(resp. $RPtw$) the rooted P-trees which arise when the edge (v, w) is deleted from Pt and has the root v(resp. w). Without loss of generality, let v be white and w be black. Fig. 6 shows the rooted P-trees in Theorem 5.

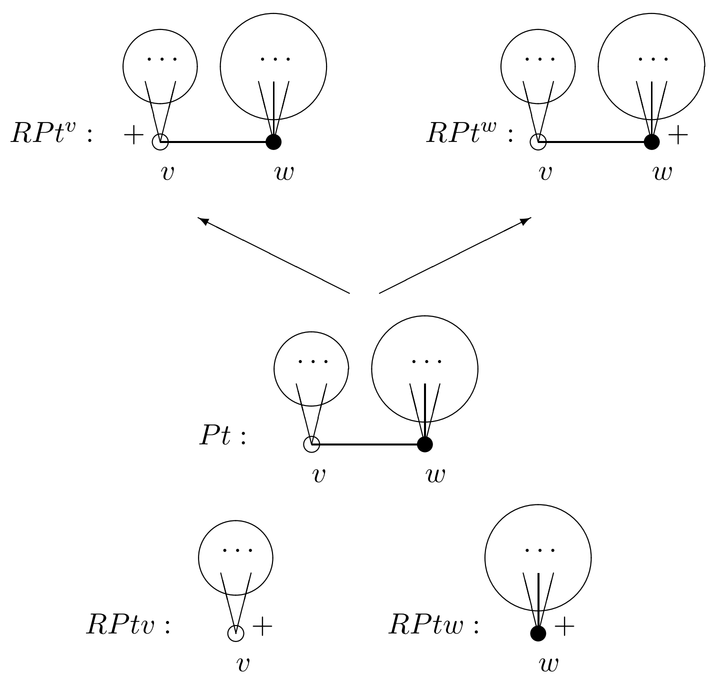

Fig. 6. Trees of Theorem 5

Theorem 5. *With the above notations, we have*

$$\frac{1}{\gamma(RPt^v)} + \frac{1}{\gamma(RPt^w)} = \frac{1}{\gamma(RPtv)\gamma(RPtw)}, \tag{23.1}$$

$$\Phi(RPt^v) + \Phi(RPt^w) = \Phi(RPtv)\Phi(RPtw) \tag{23.2}$$

when $a_s = b_1 = 0$.

Proof. By the definition of γ, we have

$$\begin{cases} \gamma(RPt^v) = n\gamma(RPtw)\left(\dfrac{\gamma(RPtv)}{\rho(RPtv)}\right), \\ \gamma(RPt^w) = n\gamma(RPtv)\left(\dfrac{\gamma(RPtw)}{\rho(RPtw)}\right). \end{cases} \tag{24}$$

Since $\rho(RPtv) + \rho(RPtw) = n$, then

$$\begin{aligned} \frac{1}{\gamma(RPt^v)} + \frac{1}{\gamma(RPt^w)} &= \frac{\rho(RPtv)}{n\gamma(RPtw)\gamma(RPtv)} + \frac{\rho(RPtw)}{n\gamma(RPtw)\gamma(RPtv)} \\ &= \frac{1}{\gamma(RPtw)\gamma(RPtv)}. \end{aligned}$$

So we get (23.1). We also have

$$\begin{cases} \Phi(RPt^v) = \displaystyle\sum_{i_v=1}^{s-1} a_{i_v}\Pi_1^{i_v} \sum_{i_w=1}^{i_v} b_{i_w}\Pi_2^{i_w}, \\ \Phi(RPt^w) = \displaystyle\sum_{i_w=1}^{s} b_{i_w}\Pi_2^{i_w} \sum_{i_v=1}^{i_w-1} a_{i_v}\Pi_1^{i_v}, \end{cases} \tag{25}$$

where $\Pi_1^{i_v}$(resp. $\Pi_2^{i_w}$) is the product of all $\Phi(RPt_b^i)$(resp. $\Phi(RPt_a^i)$), while

$$RPtv =_a [RPt_b^1, \cdots, RPt_b^{m_1}](\text{resp. } RPtw =_b [RPt_a^1, \cdots, RPt_a^{m_2}])$$

and i_v, i_w are labels of v and w respectively. $\Pi_1^{i_v}$(resp. $\Pi_2^{i_w}$) varies only according to i_v(resp. i_w). Since

$$\begin{cases} \Phi(RPtv) = \displaystyle\sum_{i_v=1}^{s-1} a_{i_v}\Pi_1^{i_v}, \\ \Phi(RPtw) = \displaystyle\sum_{i_w=1}^{s} b_{i_w}\Pi_2^{i_w}, \end{cases} \tag{26}$$

then

$$\begin{aligned} \Phi(RPtv)\Phi(RPtw) &= \sum_{i_v=1}^{s-1} a_{i_v}\Pi_1^{i_v} \sum_{i_w=1}^{s} b_{i_w}\Pi_2^{i_w} \\ &= \sum_{i_v=1}^{s-1} a_{i_v}\Pi_1^{i_v}\Big(\sum_{i_w=1}^{i_v} b_{i_w}\Pi_2^{i_w} + \sum_{i_w=i_v+1}^{s} b_{i_w}\Pi_2^{i_w}\Big) \\ &= \sum_{i_v=1}^{s-1} a_{i_v}\Pi_1^{i_v} \sum_{i_w=1}^{i_v} b_{i_w}\Pi_2^{i_w} + \sum_{i_v=1}^{s-1} a_{i_v}\Pi_1^{i_v} \sum_{i_w=i_v+1}^{s} b_{i_w}\Pi_2^{i_w}, \end{aligned}$$

and from direct computation, we have

$$\begin{aligned}\sum_{i_v=1}^{s-1} a_{i_v}\Pi_1^{i_v}\sum_{i_w=i_v+1}^{s} b_{i_w}\Pi_2^{i_w} &= \sum_{i_w=2}^{s} b_{i_w}\Pi_2^{i_w}\sum_{i_v=1}^{i_w-1} a_{i_v}\Pi_1^{i_v}\\ &= \sum_{i_w=1}^{s} b_{i_w}\Pi_2^{i_w}\sum_{i_v=1}^{i_w-1} a_{i_v}\Pi_1^{i_v}, \quad \text{when} \quad b_1=0.\end{aligned}$$

We then get (23.2).

Corollary 6. Suppose the scheme (7) with $a_s=b_1=0$ has order at least $n-1(n\geq 2)$. Then the order condition $\Phi(RPt^v)=\dfrac{1}{\gamma(RPt^v)}$ holds iff $\Phi(RPt^w)=\dfrac{1}{\gamma(RPt^w)}$ holds.

Proof. Since $\rho(RPtv),\rho(RPtw)\leq n-1$, from (18) we already have

$$\Phi(RPtv)=\frac{1}{\gamma(RPtv)},\quad \Phi(RPtw)=\frac{1}{\gamma(RPtw)}.$$

From (23), we see the corollary is obvious.

We then get the conclusion of this section:

Theorem 7. *The scheme* (7) *with* $a_s=b_1=0$ *is of order* p *iff for every P-tree* Pt *with* $\rho(Pt)\leq p$*, there exists a rooted P-tree* RPt *which arises when one of the vertices of* Pt *is considered as the root, such that* $\Phi(RPt)=\dfrac{1}{\gamma(RPt)}$ *holds.*

3. Simplified Order Conditions for Canonical RKN Methods

Let us consider the special kind of systems of second order ordinary differential equations

$$\ddot{y}=f(y), \tag{27}$$

where $y=(y^1,y^2,\cdots,y^n),\ f=(f^1,f^2,\cdots,f^n)$. (27) is equivalent to

$$\begin{bmatrix} y\\ y'\end{bmatrix}'=\begin{bmatrix} y'\\ f(y)\end{bmatrix}. \tag{28}$$

When $f(y)=\dfrac{\partial u}{\partial y}$, let $H=\dfrac{1}{2}y'^Ty'-u(y)$. Then (28) turns into a Hamiltonian system:

$$\begin{bmatrix} y\\ y'\end{bmatrix}'=\begin{bmatrix} \dfrac{\partial H(y,y')}{\partial y'}\\ -\dfrac{\partial H(y,y')}{\partial y}\end{bmatrix}. \tag{29}$$

A general s-stage RKN method for system (28) is of the form

$$\begin{cases} g_i = y_0 + c_i h y_0' + h^2 \sum_{j=1}^{s} a_{ij} f(g_j), \quad i = 1, 2, \cdots, s, \\ y_1 = y_0 + h y_0' + h^2 \sum_{j=1}^{s} \bar{b}_j f(g_j), \\ y_1' = y_0' + h \sum_{j=1}^{s} b_j f(g_j). \end{cases} \tag{30}$$

Theorem 8. *The difference scheme* (30) *is canonical iff*

$$\overline{b}_j = b_j(1 - c_j), \quad 1 \le j \le s, \tag{31.1}$$

$$b_i a_{ij} - b_j a_{ji} + \bar{b}_i b_j - b_i \bar{b}_j = b_i a_{ij} - b_j a_{ji} + b_i b_j (c_j - c_i) = 0, \quad 1 \le i, j \le s. \tag{31.2}$$

See [10–11] for the proof of Theorem 8.

Now we can define the elementary weight $\Phi(RLSt)$ corresponding to a rooted labeled S-tree. First, for convenience, we assume $RLSt$ is monotonically labeled. Later we will see this is unnecessary. In the remainder of this paper, if not otherwise pointed out, the labels of the vertices are always $j < k < l < m < \cdots$. For a monotonic labeling, the label of the root is j. Then $\Phi(RLSt)$ is a sum over the labels of all black vertices of $RLSt$; the general term of the sum is a product of

(i) b_j;

(ii) a_{kl} if the black vertex k is connected via a white son with another black vertex l;

(iii) c_k^m if the black vertex k has m white end-vertices as its sons, where an end-vertex is the vertex which has no son.

Because the elementary weight is a sum over the labels of all black vertices, it just depends on the relationship among the vertices and is independent of the labels. Choosing the monotonic labeling is then unnecessary. We see that, for two different rooted labeled S-trees: $RLSt^1, RLSt^2 \in RSt$, we have $\Phi(RLSt^1) = \Phi(RLSt^2) = \Phi(RSt)$; thus, the elementary weight for a rooted S-tree RSt is also defined.

In [12], we used the first canonical condition (31.1) in Theorem 8 to simplify the order conditions of RKN method given in [4] and got the following theorem:

Theorem 9. *A canonical RKN method* (30) *is of order p iff*

$$\Phi(RSt) = \frac{1}{\gamma(RSt)}, \textit{ for rooted } S-tree \ RSt \textit{ with } \rho(RSt) \le p.$$

Let St be an S-tree of order $n (n \ge 3)$ that has at least two black vertices. Let v and w be two black vertices of LSt connected via a white vertex u. We consider six rooted S-trees as follows. Denote by RSt^v(resp. RSt^w) the rooted S-tree obtained by regarding the vertex v(resp. w) as the root of St. Denote by RSt^{vu}(resp. RSt^{wu})

the rooted S-tree with root v(resp. w) that arises when the edge (u,w)(resp. (u,v)) is deleted from St. At last, denote by $RStv$ and $RStw$ the rooted S-trees with root at v and w respectively which arise when edges $(u,v),(u,w)$ are deleted from St. Fig. 7 shows the rooted trees of Theorem 10.

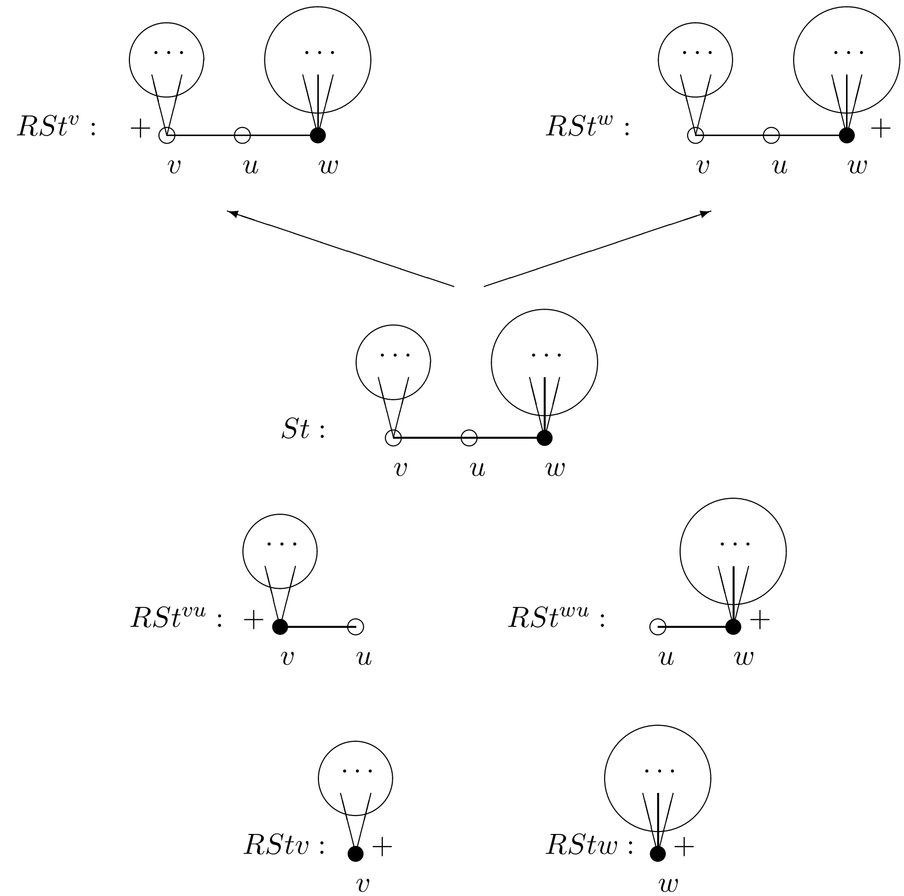

Fig. 7. Trees of Theorem 8

Theorem 10. *With the above notations, we have*

$$\frac{1}{\gamma(RSt^v)} - \frac{1}{\gamma(RSt^w)} = \frac{1}{\gamma(RSt^{vu})\gamma(RStw)} - \frac{1}{\gamma(RSt^{wu})\gamma(RStv)}. \tag{32.1}$$

And if the RKN method (30) *satisfies* (31), *then*

$$\Phi(RSt^v) - \Phi(RSt^w) = \Phi(RSt^{vu})\Phi(RStw) - \Phi(RSt^{wu})\Phi(RStv). \tag{32.2}$$

Proof. Let $\rho(RStv) = x, \rho(RStw) = y, n = \rho(St) = x + y + 1$. From the definition of γ, we have

$$\begin{cases} \gamma(RSt^v) = n\Pi_1(y+1)\gamma(RStw), \\ \gamma(RSt^w) = n\Pi_2(x+1)\gamma(RStv), \end{cases} \tag{33}$$

where Π_1(resp. Π_2) denotes the product of $\gamma(t_i)$ of the sub-trees t_i which arise when v(resp. w) is chopped from $RStv$(resp. $RStw$). Notice that $\gamma(RSt)$ is calculated as the general tree t, with the difference between the black and white vertices neglected. Then

$$\frac{1}{\gamma(RSt^v)} - \frac{1}{\gamma(RSt^w)} = \frac{1}{n}\left(\frac{\Pi_2(x+1)\gamma(RStv) - \Pi_1(y+1)\gamma(RStw)}{\Pi_2(x+1)\gamma(RStv)\Pi_1(y+1)\gamma(RStw)}\right). \tag{34}$$

Since $\gamma(RSt^{vu}) = (x+1)\Pi_1, \gamma(RSt^{wu}) = (y+1)\Pi_2$ and $\gamma(RStv) = x\Pi_1, \gamma(RStw) = y\Pi_2$, we have

$$\begin{aligned} \frac{1}{\gamma(RSt^v)} - \frac{1}{\gamma(RSt^w)} &= \frac{1}{n}\left(\frac{\Pi_2(x+1)\gamma(RStv) - \Pi_1(y+1)\gamma(RStw)}{\gamma(RSt^{vu})\gamma(RSt^{wu})\gamma(RStv)\gamma(RStw)}\right) \\ &= \frac{1}{n}\left(\frac{\Pi_1\Pi_2(x^2-y^2+x-y)}{\gamma(RSt^{vu})\gamma(RSt^{wu})\gamma(RStv)\gamma(RStw)}\right). \end{aligned} \tag{35}$$

But

$$\begin{aligned} &\frac{1}{\gamma(RSt^{vu})\gamma(RStw)} - \frac{1}{\gamma(RSt^{wu})\gamma(RStv)} \\ &= \frac{n(\gamma(RSt^{wu})\gamma(RStv) - \gamma(RSt^{vu})\gamma(RStw))}{n(\gamma(RSt^{vu})\gamma(RSt^{wu})\gamma(RStv)\gamma(RStw))} \\ &= \frac{n(\Pi_2(y+1)\Pi_1 x - \Pi_1(x+1)\Pi_2 y)}{n(\gamma(RSt^{vu})\gamma(RSt^{wu})\gamma(RStv)\gamma(RStw))} \\ &= \frac{\Pi_1\Pi_2(x+y+1)(x(y+1)-(x+1)y)}{n(\gamma(RSt^{vu})\gamma(RSt^{wu})\gamma(RStv)\gamma(RStw))} \\ &= \frac{\Pi_1\Pi_2(x^2-y^2+x-y)}{n(\gamma(RSt^{vu})\gamma(RSt^{wu})\gamma(RStv)\gamma(RStw))}. \end{aligned} \tag{36}$$

Thus we get (32.1). From the definition of Φ, we have

$$\begin{cases} \Phi(RSt^{vu}) = \sum_{i_v} b_{i_v} c_{i_v} \Pi^v, \quad \Phi(RStv) = \sum_{i_v} b_{i_v} \Pi^v \\ \Phi(RSt^{wu}) = \sum_{i_w} b_{i_w} c_{i_w} \Pi^w, \quad \Phi(RStw) = \sum_{i_w} b_{i_w} \Pi^w \end{cases} \tag{37}$$

and

$$\begin{cases} \Phi(RSt^v) = \sum_{i_v, i_w} b_{i_v} a_{i_v i_w} (\Pi^v \Pi^w), \\ \Phi(RSt^w) = \sum_{i_w, i_v} b_{i_w} a_{i_w i_v} (\Pi^v \Pi^w), \end{cases} \tag{38}$$

where Π^v(resp. Π^w) denotes part of $\Phi(RSt^v)$(resp. $\Phi(RSt^v)$) which is the sum over black vertices of $RStv$(resp. $RStw$). If (30) satisfies (31.2), then we get

$$\begin{aligned}\Phi(RSt^v) - \Phi(RSt^w) &= \sum_{i_v, i_w} (b_{i_v} a_{i_v i_w} - b_{i_w} a_{i_w i_v}) \Pi^w \Pi^v \\ &= \sum_{i_v, i_w} b_{i_v} b_{i_w} (c_{i_v} - c_{i_w}) \Pi^v \Pi^w \\ &= \sum_{i_v} b_{i_v} c_{i_v} \Pi^v \sum_{i_w} b_{i_w} \Pi^w - \sum_{i_w} b_{i_w} c_{i_w} \Pi^w \sum_{i_v} b_{i_v} \Pi^v \\ &= \Phi(RSt^{vu}) \Phi(RStw) - \Phi(RSt^{wu}) \Phi(RStv).\end{aligned}$$

We have finished the proof of (32.2).

The following corollary is obvious.

Corollary 11. Suppose that the method (30) satisfying (31) has order at least $n-1$, with $n \geq 3$. If RSt^v and RSt^w are different rooted S-trees of order n, then the standard order condition $\Phi(RSt^v) = \dfrac{1}{\gamma(RSt^v)}$ holds if and only if $\Phi(RSt^w) = \dfrac{1}{\gamma(RSt^w)}$ holds.

So we get the conclusion of this section:

Theorem 12. *The RKN method* (30) *satisfying* (31) *is of order p, iff for every S-tree St, there exists a rooted S-tree RSt^v which arises when a black vertex v of St is highlighted as the root, such that $\Phi(RSt^v) = \dfrac{1}{\gamma(RSt^v)}$.*

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