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Abstract. The main result in this paper is that an infinite subset of $(6N \times 6N)$ symplectic matrices is related to the class of spanning binary trees with N leaves. The linear canonical transformations connected with these symplectic matrices, provide a generalization and unified treatment of the well-known Jacobi coordinates in celestial mechanics. It is essentially this correspondence with trees, that make them so useful in problems where the relative separations between N particles is important; for example, the study of clusters. The correspondence with graph theory also provides elegant methods to classify and enumerate these special symplectic matrices, which yields the result that for a given N, there are $4(2N-3)!$ of them.

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I. Introduction. The application of graph theory to mathematical physics has a long and illustrious tradition. Some of the highlights of this endeavor are Feynman diagrams in Quantum Field Theory [1], and Mayer's Cluster Expansion in Statistical Mechanics [2].

The purpose of this paper is to present a new application of graph theory to an old field, namely canonical transformations for N-body Problems in Celestial Mechanics, [3, 4, 5, 6]. Specifically, it shall be shown that spanning binary trees* with N leaves, are related to $6N \times 6N$ symplectic matrices. Linear canonical transformations for the hamiltonians of celestial mechanics are characterized completely by symplectic matrices, $\mathbf{M}$ such that

$$\mathbf{M}^t\mathbf{J}\,\mathbf{M} = \mathbf{J}\,, \qquad \mathbf{J} = \begin{bmatrix} \mathbf{0} & \mathbf{I}_N \\ -\mathbf{I}_N & \mathbf{0} \end{bmatrix}. \tag{1}$$

In particular, for the transformation,

$$\begin{aligned} \mathbf{Q} &= \mathbf{Q}(\mathbf{q},\mathbf{p}) \\ \mathbf{P} &= \mathbf{P}(\mathbf{q},\mathbf{p}) \end{aligned} \tag{2}$$

where all vectors are elements of $\mathbf{R}^{3N}$, the Jacobian matrix has four blocks,

$$\mathbf{M} = \begin{bmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{bmatrix} \tag{3}$$

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*All the relevant graph-theoretical concepts are in italics and collected in the appendix, for the convenience of the reader. For more details, the reader should consult Biggs [7] and Gibbons [8].

where $\mathbf{A}, \mathbf{B}, \mathbf{C}, \mathbf{D}$ are $3N \times 3N$ real constant matrices. The symplectic condition can be easily shown to be equivalent to

$$\text{(4.a)} \qquad \mathbf{A}^t\mathbf{C}\ ,\ \mathbf{B}^t\mathbf{D} \quad \text{are symmetric matrices}$$

$$\text{(4.b)} \qquad \mathbf{A}\mathbf{D}^t - \mathbf{C}\mathbf{B}^t = \mathbf{I}_{3N}$$

In this paper, only symplectic matrices of the form

$$\text{(5)} \qquad \mathbf{M} = \begin{bmatrix} \mathbf{A} & \mathbf{O} \\ \mathbf{O} & \mathbf{D} \end{bmatrix}, \qquad \mathbf{A} \neq \mathbf{D}.$$

which correspond to transformations of the type

$$\text{(6)} \qquad \mathbf{Q} = \mathbf{Q}(\mathbf{q}), \qquad \mathbf{P} = \mathbf{P}(\mathbf{p})$$

are discussed. For such matrices, the condition (4a) is obviously satisfied and condition (4b) becomes

$$\text{(7)} \qquad \mathbf{A}\mathbf{D}^t = \mathbf{I}_{3N}.$$

The well-known Jacobi coordinates in celestial mechanics (discussed in the literature only for special cases such as the 3-body Problem) fall into the above class of canonical transformations, (6) [3]. These coordinates are useful precisely because they represent relative distances between the particles in N-body problems. Not all matrices of the form, (5) give interesting or useful linear transformations.

This paper describes a procedure for generating an infinite subset of symplectic matrices having the form (5). The procedure is graph-theoretic and the point of departure is the association of a *complete* graph $\mathbf{K}_N$ with N-body hamiltonians that describe 2-body interactions between all pairs of particles.

Starting from $\mathbf{K}_N$, the procedure creates $(N-1)$ additional vertices in a well-defined way. Then a *spanning binary tree* with $(2N-1)$ vertices, in which the *leaves* are exactly the original vertices in $\mathbf{K}_N$, is constructed. There are in fact many such *trees* that can be generated from $\mathbf{K}_N$, for a given N. Part of this paper concerns the classification problem, that is, what are the natural sub-classes of such binary trees?

Each binary tree generated by this procedure defines a set of symplectic matrices, (5) according to explicit formulae that depend on the topological structure of the tree. The classification referred to above, therefore induces a classification of the corresponding symplectic matrices. It turns out that this infinite subset of symplectic matrices having the form, (5) defines useful linear canonical transformations by virtue of their construction in terms of trees. In fact, they represent a significant generalization of the so-called Jacobi coordinates.

The isolated cases of Jacobi coordinates discussed in the literature, are shown to be canonical transformations by verifying separately in each case that condition (7) holds. Here, a unified treatment is given that combines the construction, classification, and enumeration of the generalized Jacobi coordinates, in addition to a direct proof of their symplectic nature, (7).

Besides the construction and classification of the binary trees outlined above, the second part of this paper concerns the enumeration problem, that is, how many binary trees are there in each sub-class and also, how many are there altogether, for a given positive integer, N? Of course, the answers to these questions also give the number of symplectic matrices.

In section II, the procedure for the construction and classification of the binary trees is given; in section III, the explicit formulae that define symplectic matrices in terms of the topological structure of these trees, are discussed. Section IV is devoted to the proof of the main result that all the binary trees constructed by this procedure, give symplectic matrices of the type, (5) via the formulae in section III. Finally, section V treats the enumeration problem mentioned above.

In a previous paper [9], symplectic matrices of the form.

$$\mathbf{M} = \begin{bmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{A} \end{bmatrix}$$

are discussed but the proof there is restricted to a sub-class of binary trees.

II. Construction and Classification. The introduction of graph-theoretic concepts in the study of N-body problems is based on the following correspondence between a complete graph, $\mathbf{K}_N$ and N-body hamiltonians

$$H = \sum_{j=1}^{N} \frac{|\mathbf{p}_j|^2}{2m_j} - U(\mathbf{q}) \tag{2.1}$$

where $\mathbf{q} = (\mathbf{q}_1, \mathbf{q}_2, \ldots, \mathbf{q}_N)$ and $\mathbf{p} = (\mathbf{p}_1, \ldots, \mathbf{p}_N)$ are vectors in $\mathbf{R}^{3N}$, m_j are the masses of the particles and $|\mathbf{p}_j|^2$ is given by the euclidean norm in $\mathbf{R}^3$. The general potential function has the form of a sum over all unequal pairs (j,k) of integers from 1 to N,

$$U(\mathbf{q}) = G \sum_{j \neq k}^{N} \frac{m_j m_k}{|\mathbf{q}_j - \mathbf{q}_k|^l} \tag{2.2}$$

where G is a real constant, and

$$|\mathbf{q}_j - \mathbf{q}_k|^l \equiv \left[\left(q_j^{(1)} - q_k^{(1)}\right)^2 + \left(\mathbf{q}_j^{(2)} - \mathbf{q}_k^{(2)}\right)^2 + \left(\mathbf{q}_j^{(3)} - \mathbf{q}_k^{(3)}\right)^2 \right]^{l/2}. \tag{2.3}$$

l is a real number greater than zero and the Newtonian case is obtained when $l = 1$. From (2.2), it is easy to see that if the vertices of $\mathbf{K}_N$ represent the positions of the particles, $\mathbf{q}_j$, then the edges can be profitably chosen to represent the terms in the potential function.

The procedure for the construction of the spanning binary trees with $(2N-1)$ vertices, in which all the *leaves* are the original vertices in $\mathbf{K}_N$, consists of two parts: (a) an *averaging* step that defines a binary operation INTER, based on which, $(N-1)$ virtual vertices are added to the original ones in $\mathbf{K}_N$ (b) each virtual vertex $\mathbf{V}_j$ is then linked by *edges* to the vertices which are the arguments of INTER that resulted in $\mathbf{V}_j$.

The binary operation, INTER is given by

$$\begin{aligned} \mathbf{V} &= INTER(\mathbf{A}, \mathbf{B}) \\ &= \frac{m(\mathbf{A})\ \mathbf{A} + m(\mathbf{B})\mathbf{B}}{m(\mathbf{A}) + m(\mathbf{B})} \end{aligned} \tag{2.4}$$

where $\mathbf{V} = \mathbf{V}_j$ is a new virtual vertex and the arguments $\mathbf{A}, \mathbf{B}$ can be either a previously generated virtual vertex, e.g. $\mathbf{V}_h$ for some $h < j$ or one of the original vertices in $\mathbf{K}_N$, e.g. $\mathbf{q}_j, j = 1, \ldots, N$; the mass function $m(\cdot)$ assigns a real number to a new vertex $\mathbf{V}$ in the following way:

$$m(\mathbf{V}) = m(\mathbf{A}) + m(\mathbf{B}) \tag{2.5}$$

where $\mathbf{V}, \mathbf{A}, \mathbf{B} \in \mathbf{R}^3$ are the same as in (2.4). The mass function gives the correct masses, m_j when applied to $\mathbf{q}_j$, $j = 1, \ldots, N$.

This operation is governed by the rules:

(i) vertices (both virtual or original) can only be used *once* as arguments in INTER.

(ii) to begin, $k \le \left[\frac{N}{2}\right]$ *disjoint* edges in $\mathbf{K}_N$ are preselected to produce the first k virtual vertices, $\mathbf{V}_j$ where $1 \le j \le k$.

(iii) the process ends when there are no more eligible pair of vertices (original or virtual) to use as arguments of INTER.

The original vertices, $\mathbf{q}_j$ in $\mathbf{K}_N$ are said to be in tier 0 while the first k virtual vertices in rule (ii), are said to be in tier 1; virtual vertices generated by subsequent applications of INTER are said to be in tiers ≥ 2, according to the number of times INTER have been used.

After relabelling (by permutations on N integers) of the tier 0 vertices, the tier 1 vertices, can, without loss of generality, be taken to be

$$\begin{aligned} \mathbf{V}_1 &= INTER\ (\mathbf{q}_1, \mathbf{q}_2) \\ \mathbf{V}_2 &= INTER\ (\mathbf{q}_3, \mathbf{q}_4) \\ &\ \vdots \\ \mathbf{V}_k &= INTER\ (\mathbf{q}_{2k-1}, \mathbf{q}_{2k}) \end{aligned} \tag{2.6}$$

For N large compared to the number, k of tier 1 vertices, (2.6), there are clearly many ways to generate the virtual vertices in tiers ≥ 2.

When all the virtual vertices, $\mathbf{V}_j$ have been created, a graph is constructed by putting edges between each $\mathbf{V}_j$ and the two arguments of INTER, which were used to create $\mathbf{V}_j$.

LEMMA 2.1. *Every graph G, generated by INTER, according to the rules on page 4 , have the following properties:*

(a) *G is a binary tree, and the **descendents** of a vertex, V are the two arguments of INTER that created V*
(b) *it consists of $(2N-1)$ vertices and is a spanning tree*
(c) *the leaves (vertices of degree one) are in one-to-one correspondence with the tier 0 vertices or original vertices in $\mathbf{K}_N, \mathbf{q}_j,\ j = 1, \ldots, N$*
(d) *the root of G is $\mathbf{V}_{N-1}$, the virtual vertex in the highest tier or the one generated last.*
(e) *all other virtual vertices (except the root) have degree 3.*

Proof.

(a) The fact that G is a tree follows from rule (i) for INTER, which states that the tier 0 vertices and all subsequent virtual vertices can only be used once in INTER. Therefore there can be no ***circuits*** in G, and it must be a tree. It is a ***binary*** tree because the operation that generates it, is a binary operation which takes two arguments (vertices) and creates a new virtual vertex. The two arguments are linked by edges to the new vertex and are thus the ***descendents*** of the vertex being created.
(b) G is a spanning tree because rule (iii) for INTER states that the process for generating it stops ***only if*** there are no more eligible pairs of vertices that can serve as arguments of INTER. For, if there are unconnected components in the tree, then there must be vertices that can be used in INTER. The fact that when the process stops, the end product is a spanning tree with $(N-1)$ additional (virtual) vertices follows from the following simple result, Lemma 2.2. Property (e) follows directly from the fact that G is a spanning binary tree.

LEMMA 2.2. *If a binary spanning tree, T has m leaves (degree 1 vertices), then it has $(m-1)$ additional vertices of degrees 2 and 3.*

Proof. The proof is by mathematical induction on m. The result clearly holds for a binary tree with 2 leaves. Suppose the result is valid for binary trees with $(m-2)$ leaves. Remove a pair of leaves from T so that the resulting tree, T' is still a binary tree, with $(m-1)$ leaves. The result states that there are $(m-2)$ additional vertices in T' with higher degrees. Now putting back the leaves removed in the previous step, a leave in $\mathbf{T}'$ is converted to a vertex of degree 3 and therefore, there are $(m-1)$ vertices with degree > 1.

(c) This is a direct consequence of rule (i) for the construction process.

(d) Because the spanning trees are constructed from the leaves (tier 0 vertices) up, the last virtual vertex created is the root and it must therefore be $\mathbf{V}_{N-1}$ and have degree 2.

The multitude of spanning trees generated by the above procedure, can be conveniently classified by the number of virtual vertices in each tier. For example, suppose a tree constructed from $\mathbf{K}_N$ (with N tier 0 vertices) has k tier 1 vertices, l tier 2 vertices, m tier 3 and so on until the $(n-1)$-th virtual vertex, $\mathbf{V}_{N-1}$ has been accounted for. Then this tree belongs to the sub-class, $\mathbf{G}^{(N)}_{k,l,m,\dots,1}$ where the last subscript must be one because there can only be one virtual vertex in the highest tier for the tree, namely the *root*, $\mathbf{V}_{N-1}$.

Later in this paper, a specific label for each tree will be derived, and used to enumerate the total number of such trees for a given N.

2.1 The sub-class $G_{k,1,1,\dots,1}(N)$.. To indicate the variety and richness of these trees, the sub-class $\mathbf{G}_{k,1,1,\dots,1}(N)$ will be examined in greater details. In fact, it shall be clear later, that the trees in the other sub-classes can be derived from those in this sub-class.

Now, there are so many trees even in this sub-class, that it will be convenient to organize them in the way they are constructed, according to the general rules laid down earlier. For this purpose an associated tree $\mathbf{A}^k_N$ is introduced:

(i) the root of $\mathbf{A}^k_N$ is labelled 1 to represent $\mathbf{V}_1$.

(ii) the branches of $\mathbf{A}^k_N$ code the creation of virtual vertices in tiers ≥ 2, after the tier 1 vertices, $\mathbf{V}_j$ for $j = 1, \dots, k$ have been generated as in (2.6).

(iii) because there is one virtual vertex in each tier ≥ 2 (for the sub-class $\mathbf{G}_{k,1,1,\dots,1}(N)$), and the general rules stipulate that these vertices, $\mathbf{V}_{k+1}$ to $\mathbf{V}_{N-1}$, are created in the order of their subscripts, the vertices of $\mathbf{A}^k_N$ below the root, are labelled $(k+1)$ to $(N-1)$ in the same order on each branch.

(iv) an edge of $\mathbf{A}^k_N$ is labelled by a boxed quantity, e.g. $\boxed{\mathbf{V}_2} = (1, K+1)$ where the first member of the pair denotes the *upper* vertex in the edge (relative to the root); in this example, the operation, $\mathbf{V}_{k+1} = INTER\ (\mathbf{V}_1, \mathbf{V}_2)$ is encoded.

(v) the *lower* vertex in the edge, always represent the new virtual vertex created by the encoded INTER operation, while the upper vertex represents the first argument in the same operation.

(vi) the quantity in the box, always represent the second argument in the INTER operation that is encoded; infact, this quantity consists of only the tier O vertices, $\mathbf{q}_j, 2k+1 \leq j \leq N$ and the tier 1 vertices, $\mathbf{V}_j, j = 1, \dots, k$.

A simple example, $\mathbf{A}_5^2$ is now given to illustrate the concept of an associated tree (cf. fig. 1). In this case, the trees in the sub-class, $\mathbf{G}_{2,1,1}(5)$, are completely characterized. It should be noted that $k = 2$, is the maximum number of tier 1 vertices, or equivalently, disjoint edges in the complete graph, $\mathbf{K}_5$.

First, the tier 1 vertices are generated (cf. (2.6)),

$$\begin{aligned} \mathbf{V}_1 &= INTER\,(\mathbf{q}_1, \mathbf{q}_2) \\ \mathbf{V}_2 &= INTER\,(\mathbf{q}_3, \mathbf{q}_4) \end{aligned} \tag{2.7}$$

The root of $\mathbf{A}_2^5$ is labelled 1, after $\mathbf{V}_1$. From the root, there are two distinct ways to generate the tier 2 vertex, $\mathbf{V}_3$. On the right branch, depicted in fig. 1c,

$$\mathbf{V}_3 = INTER\,(\mathbf{V}_1, \mathbf{V}_2)$$

and on the left, depicted in fig. 1b,

$$\mathbf{V}_3 = INTER(\mathbf{V}_1, \mathbf{q}_5).$$

These operations are encoded in the edges descending from the root,

$$\begin{aligned} \boxed{\mathbf{V}_2} &= (1,3) \\ \boxed{\mathbf{q}_5} &= (1,3) \end{aligned}$$

The next virtual vertex, in tier 3, is $\mathbf{V}_4$ and it is given by

$$\begin{aligned} \mathbf{V}_4 &= INTER\,(\mathbf{V}_3, \mathbf{q}_5) \\ \mathbf{V}_4 &= INTER\,(\mathbf{V}_3, \mathbf{V}_2) \end{aligned}$$

on the right and left branches respectively. Since there are no more arguments for INTER, the process stops and all four virtual vertices in the two spanning trees, $\mathbf{G}_{2,1,1}^s(5)$, $s = 1, 2$ have been generated. Clearly, all the tier 0 vertices, $\mathbf{q}_j$, $j = 1, \ldots, 5$, and the tier 1 vertices, $\mathbf{V}_j, j = 1, 2$, have been used only once, thereby satisfying the rules that govern INTER.

It remains to discuss the index $s = 1, 2$ in the labels $\mathbf{G}_{k,1,1}^s(5)$. The left and right branches of $\mathbf{A}_5^2$ have the respective path (edge) representations,

$$\begin{aligned} \mathbf{G}_{2,1,1}^1(5) &= \left\{\boxed{\mathbf{q}_5}, \boxed{\mathbf{V}_2}\right\} &= \{0\ \ 1\} \\ \mathbf{G}_{2,1,1}^2(5) &= \left\{\boxed{\mathbf{V}_2}, \boxed{\mathbf{q}_2}\right\} &= \{1\ \ 0\} \end{aligned}$$

The index s in the above labels, takes the value of the binary number obtained when the path representation is put in binary form, where 0 denotes a tier 0 vertex, and 1 denotes a tier 1 vertex.

Earlier, in (2.6), the relabelling of the tier 0 vertices by a permutation on N integers, is mentioned. Such a relabelling has the effect of changing the actual $\mathbf{A}_N^k$ but the resulting spanning binary trees differs only superficially. In other words, they have the same topological structure. Indeed, two trees generated by the same branch of $\mathbf{A}_N^k$ (defined in terms of the binary form), but differing by such a permutation, are *equivalent*. Thus, this relabelling defines equivalence classes of spanning trees, which are completely characterized by the binary representation of the branches of $\mathbf{A}_N^k$.

The binary representation of a branch, defines the *order* in which the tier 1 vertices *vis–a–vis* the tier 0 vertices, appears as the second argument in INTER. It gives a convenient algorithm to enumerate the number of branches (equivalence classes) in $\mathbf{A}_N^k$. Since only

$$(2.8) \qquad \begin{array}{ll} (N-2k) & \text{tier } 0 \text{ vertices and,} \\ (k-1) & \text{tier 1 vertices} \end{array}$$

can appear in the path representations according to property (vi) of $\mathbf{A}_N^k$, the following result is obtained immediately,

THEOREM 2.1. *there are* $\binom{N-k-1}{k-1}$ *branches in* $\mathbf{A}_N^k$ *or equivalence classes of spanning binary trees,* $\mathbf{G}^s_{k,1,\ldots,1}(N)$ *in the sub-class* $\mathbf{G}_{k,1,1,\ldots,1}(N)$.

It is important to note that the proof of the main result depends only on the characteristics of the equivalence class and not on the individual member trees.

2.2 Other Sub-classes, $\mathbf{G}_{k,l,m,\ldots,1}(N)$. As mentioned earlier, a procedure that generates the trees in the other sub-classes from those in $\mathbf{G}_{k,1,\ldots,1}(N)$ exists. This procedure iteratively "grows" additional *branches* and *leaves* on a given tree, $\mathbf{G}^s_{k,1,\ldots,1}(N)$ from the previous sub-class. It is illuminating to describe this procedure in terms of examples from the sub-class, $G_{2,2,1,1}$ (7) (cf. fig. 2). On each of the two trees in $\mathbf{G}_{2,1,1}$ (5), one adds two *leaves* to the vertex labelled $\mathbf{q}_1$, and then another two *leaves* to the vertex labelled $\mathbf{q}_4$ (or alternatively $\mathbf{q}_3$). Then the first two *leaves* added are now labelled $\mathbf{q}_1$ and $\mathbf{q}_6$ while the old $\mathbf{q}_1$ is now a tier 1 virtual vertex, labelled $\mathbf{V}_5$. The next pair of *leaves* added are now labelled $\mathbf{q}_4$ and $\mathbf{q}_7$, while the old tier 0 vortex, $\mathbf{q}_4$ is now a tier 1 vertex, $\mathbf{V}_6$. In this process, the old tier 1 vertices, $\mathbf{V}_1$ and $\mathbf{V}_2$ have turned into tier 2 vertices, of which there are now two. This accounts for the index $l = 2$, which represents the fact that there are now two tier 2 vertices.

Note that the leaves of the new trees, $\mathbf{G}^s_{2,2,1,1}(7)$, $s = 1, 2$ are not labelled according to the canonical order in (2.6). This can be easily fixed by a relabelling of the leaves (tier 0 vertices) via a suitable permutation on the first seven positive integers.

This process can clearly be repeated to generate the trees in other sub-classes. Since this interesting relation between the first sub-class, $\mathbf{G}_{k,1,\ldots,1}(N)$ and the other sub-classes does not play a crucial role in the proof of the main result, further discussion of it is not warranted, except for the final remark that, it provides a different way to classify the spanning binary trees.

III. Symplectic Matrices. This section discusses the set of explicit formulae that generates symplectic matrices (5) from each spanning binary tree. First, let the two *descendents* of a virtual vertex, $\mathbf{V}_j$ be

$$\begin{aligned} \text{ARG}\,1(j) &= \text{1st argument in INTER that generated, } \mathbf{V}_j \\ \text{ARG}\,2(j) &= \text{2nd argument in the same operation.} \end{aligned} \tag{3.1}$$

In other words,

$$\mathbf{V}_j = INTER(\,\text{ARG}\,1(j),\ \text{ARG}\,2(j)) \tag{3.2}$$

and the mass function (2.5) is

$$m(\mathbf{V}_j) = m(\,\text{ARG}\,1(j)) + m(\,\text{ARG}\,2(j)). \tag{3.3}$$

To each virtual vertex, $\mathbf{V}_j$ (in tiers ≥ 1) in the binary tree, there belongs corresponding "rows" in the matrices $\mathbf{A}$ and $\mathbf{D}$, given explicitly by

$$\mathbf{Q}_j = \text{ARG}\,2(j) - \text{ARG}\,1(j) \tag{3.4}$$

$$\mathbf{P}_j = \left[\frac{m(\,\text{ARG}\,1(j))\cdot m(\,\text{ARG}\,2(j))}{m(\mathbf{V}_j)}\right] \times \left(\dot{\text{ARG}}\ 2(j) - \dot{\text{ARG}}\ 1(j)\right) \tag{3.5}$$

respectively. In the above, ARG $1(j)$, ARG $2(j)$, $\mathbf{Q}_j, \mathbf{P}_j$ are vectors in $\mathbf{R}^3$, and $\dot{\text{ARG}}1(j)$, $\dot{\text{ARG}}2(j)$ denote the time derivatives of the corresponding vector quantities. The following formula completes the above $(N-1)$ in (3.4) and (3.5),

$$\mathbf{Q}_N = \frac{\sum_{j=1}^{N} m_j \mathbf{q}_j}{\sum_{j=1}^{N} m_j} \tag{3.6a}$$

$$\mathbf{P}_N = \frac{\sum_{j=1}^{N} \mathbf{p}_j}{\sum_{j=1}^{N} m_j} \tag{3.6b}$$

The arguments ARG $1(j)$, ARG $2(j)$ are linear combinations of the tier 0 vertices, $\mathbf{q}_j \in \mathbf{R}^3, j = 1, \ldots, N$ while the time derivatives $\overset{\bullet}{\text{ARG}}\ 1(j)$, $\overset{\bullet}{\text{ARG}}\ 2(j)$ can be written as linear combinations of the conjugate momenta by the substitution,

$$\frac{\mathbf{p}_j}{m_j} = \overset{\bullet}{q}_j. \tag{3.7}$$

Therefore, (3.4) and (3.6a) define a real linear transformation from $\{\mathbf{q}_j\} \in \mathbf{R}^{3N}$ to new (Jacobi) coordinates, $\{\mathbf{Q}_j\} \in \mathbf{R}^{3N}$. At the same time, (3.5) and (3.6b) give a real linear transformation from $\{\mathbf{p}_j\} \in \mathbf{R}^{3N}$ to $\{\mathbf{P}_j\} \in \mathbf{R}^{3N}$. Indeed, the first transformation defines the $3N \times 3N$ real constant matrix, $\mathbf{A}$, and the second defines the matrix, $\mathbf{D}$ in $\mathbf{M}$, (5).

The following example demonstrates how a symplectic matrix can be derived from the graph, $\mathbf{G}^1_{2,1,1}(5)$ (cf. fig. 1b) by using the above explicit formulae. To each virtual vertex in this graph, there belongs a row in the matrix,

$$\mathbf{A} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 1 & 0 \\ -\frac{m_1}{m_1+m_2} & -\frac{m_2}{m_1+m_2} & 0 & 0 & 1 \\ \frac{-m_1}{m_1+m_2+m_5} & \frac{-m_2}{m_1+m_2+m_5} & +\frac{m_3}{m_3+m_4} & \frac{+m_4}{m_3+m_4} & \frac{-m_5}{m_1+m_2+m_5} \\ \frac{m_1}{\sum_{j=1}^{5} m_j} & \frac{m_2}{\sum m_j} & \frac{m_3}{\sum m_j} & \frac{m_4}{\sum m_j} & \frac{m_5}{\sum m_j} \end{bmatrix} \tag{3.8}$$

and a corresponding row in the matrix,

(3.9)
$$\begin{bmatrix} \left[\frac{m_1 m_2}{m_1+m_2}\right] & \left(\frac{-\mathbf{1}}{m_1} \quad \frac{\mathbf{1}}{m_2} \quad \mathbf{0} \quad \mathbf{0} \quad \mathbf{0}\right) \\ \left[\frac{m_3 m_4}{m_3+m_4}\right] & \left(\mathbf{0} \quad \mathbf{0} \quad \frac{-\mathbf{1}}{m_3} \quad \frac{\mathbf{1}}{m_4} \quad \mathbf{0}\right) \\ \left[\frac{(m_1+m_2)m_5}{m_1+m_2+m_5}\right] & \left(\frac{-\mathbf{1}}{m_1+m_2} \quad \frac{-\mathbf{1}}{m_1+m_2} \quad \mathbf{0} \quad \mathbf{0} \quad \frac{\mathbf{1}}{m_5}\right) \\ \left[\frac{(m_1+m_2+m_5)(m_3+m_4)}{\sum_{j=1}^{5} m_j}\right] & \left(\frac{-\mathbf{1}}{m_1+m_2+m_5} \quad \frac{-\mathbf{1}}{m_1+m_2+m_5} \quad \frac{\mathbf{1}}{m_3+m_4} \quad \frac{\mathbf{1}}{m_3+m_4} \quad \frac{-\mathbf{1}}{m_1+m_2+m_5}\right) \\ \left[\frac{1}{\sum_{j=1}^{5} m_j}\right] & \left(\mathbf{1} \quad \mathbf{1} \quad \mathbf{1} \quad \mathbf{1} \quad \mathbf{1}\right) \end{bmatrix}$$

Each (bold) entry in the above matrices represents a 3×3 diagonal matrix, for examples,

$$-\mathbf{1} \equiv \begin{bmatrix} -1 & O & O \\ O & -1 & O \\ O & O & -1 \end{bmatrix}, \quad \frac{\mathbf{1}}{m_2} \equiv \begin{bmatrix} m_2^{-1} & O & O \\ O & m_2^{-1} & O \\ O & O & m_2^{-1} \end{bmatrix}$$

The symplectic matrix, **M** that consists of **A** and **D**, defines a linear canonical transformation for 5-body problems in celestial mechanics. It gives an example of the Jacobi coordinates.

IV. Main Result. The main result states that:

THEOREM 4.1. *For a given N, all the spanning binary trees, constructed above define symplectic matrices,* **M** *which have the form (5), through the formulae (3.4), (3.5) and (3.6).*

The proof of this result depends crucially on the topological structure of the spanning binary trees, although the explicit formulae in section III are apparently given in terms of the actual positions of the virtual vertices which are generated by applications of INTER. In broad terms, there are two parts in the verification of the symplectic condition, (7):

(i) the first part consists of making sure that corresponding rows of the matrices **A** and **D** have inner product equal to one,

(ii) the second part consist of verifying that non-corresponding rows (e.g. row 2 of $\mathbf{A}$ and row 3 of $\mathbf{D}$) are orthogonal.

The first depends more on the actual distance relations between the vertices which are completely prescribed in the construction process. On the other hand, the second part (as will be shown) depends rather on the topological structure of the trees.

A preliminary to the proof of theorem 4.1 will consist of steps in the following schema:

$$
\begin{tikzcd}
\mathbf{G}_{k,l,m,\ldots,1}(N) \arrow[rr, "(3.4)\text{ to }(3.6)"] \arrow[d] & & \mathbf{M}\,(6N \times 6N) \\
\mathbf{G}'_{k,l,m,\ldots,1}(N) \arrow[rr] & & H - \text{matrix} \arrow[u]
\end{tikzcd}
\tag{4.1}
$$

which summarizes the detailed analysis of the construction algorithm, (3.4) to (3.6) in terms of the topological structure of the trees. The meaning of the above schema will now be explained. Each tree in the sub-class, $\mathbf{G}_{k,l,m,\ldots,1}$ (this labels are used to denote the typical sub-class) is constructed by INTER and thus embodies the metrical relations mentioned above. To such a tree, one can associate an underlying topological tree, which represents only the connectivity of the graph (c.f. the diagrams, fig. 1 and 2). These underlying trees are labelled by the primed symbols. For each underlying tree, which again are spanning binary trees with leaves consisting of the tier 0 vertices, one can construct a N by N matrix, called the H-matrix. The last step in the above schema involves the relation between the H-matrix and the matrices $\mathbf{A}$ and $\mathbf{D}$ which make up $\mathbf{M}$.

Once all the links in the above schema are in place, the verification of condition (7) for $\mathbf{M}$ can be obtained essentially by showing that the rows of the H-matrix form an orthogonal set. First, the definition of the H-matrix will be discussed. To each virtual vertex in the tree (henceforth the underlying tree will be called tree for short), there belongs a row in the H-matrix. For example, the first k rows correspond to the k tier 1 vertices in the same order, and so on; the $(N-1)$-th row corresponds to the root (virtual vertex in the highest tier). From Lemma 2.1 and the discussion in section III, it is clear that the pair of descendents of a virtual vertex, $\mathbf{V}_j$ in the binary tree, corresponds to ARG $1(j)$ and ARG $2(j)$, (3.1). These quantities are, as mentioned earlier, linear combinations of the tier 0 vertices, $\mathbf{q}_j$, $j = 1, \ldots, N$.

Define the sets,

(4.2)

$$\chi_1(j) = \left\{ \text{integers } r \text{ from 1 to } N \text{ such that } \mathbf{q}_r \text{ enters in the definition of ARG}\,1(j) \right\}$$

$$\chi_2(j) = \left\{ \text{integers } r \text{ from 1 to } N \text{ such that } \mathbf{q}_r \text{ enters in the definition of ARG}\,2(j) \right\}$$

$$\chi(j) = \chi_1(j) \cup \chi_2(j)$$

Note that $\chi_1(j) \cap \chi_2(j) = \emptyset$ because rule (i) in the construction process stipulates that the tier 0 vertices can be used only once in INTER. In words, the set $\chi(j)$ represents the tier 0 vertices that are connected to virtual vertex $\mathbf{V}_j$ but are located *lower* in the tree.

The j-th row in the H-matrix is now given in terms of the sets, (4.2):

$$H_{jr} = \begin{cases} 1 & \text{if } r \in \chi_2(j) \\ -1 & \text{if } r \in \chi_1(j) \\ 0 & \text{if } r \notin \chi(j) \end{cases} \tag{4.3}$$

Anticipating the fact that $\mathbf{A}, \mathbf{D}$ are to be viewed as $\mathbf{N} \times \mathbf{N}$ matrices with each element a diagonal 3×3 matrix, the above H-matrix is augmented by a row of ones, that is,

$$H_{Nr} = 1 , \qquad \forall \ r = 1, \ldots, N. \tag{4.4}$$

The above operations complete the definition of the H-matrix for spanning binary trees. Next the relation between the H-matrix and the matrices $\mathbf{A}, \mathbf{D}$ (which are to be viewed as $N \times N$ matrices, as explained above) is discussed. The explicit formulae (3.4), (3.5) and (3.6) for writing down the transformation matrix $\mathbf{M}$, combined with the earlier observation that the arguments of INTER, (3.1) are linear combinations of $\mathbf{q}_j, j = 1, \ldots, N$, imply that the H-matrix is just the *occupancy* matrix for $\mathbf{A}$ and $\mathbf{D}$. Because of the way they are constructed (see example in section III), $\mathbf{A}$ and $\mathbf{D}$ have the same occupancy properties. It is therefore sufficient to discuss $\mathbf{A}$. The occupancy matrix of $\mathbf{A}$ is a $N \times N$ matrix of 0, and ± 1. The (j, r)-th element of this matrix is

$$\begin{cases} 1 & \text{if the corresponding element in } \mathbf{A} \text{ is a positive matrix,} \\ -1 & \text{if } A_{jr} \text{ is a negative matrix,} \\ 0 & \text{if } A_{jr} \text{ is unoccupied or zero.} \end{cases} \tag{4.5}$$

All the components of the schema, (4.1) have now been introduced.

The last step in (4.1) involves the detailed structure of the matrices $\mathbf{A}$ and $\mathbf{D}$ that make up the symplectic matrix, $\mathbf{M}$. In the following discussion, the structure of $\mathbf{A}$ and D will be analyzed with the help of the H-matrix (the typical row in each group below is always called the j-th row):

(1) the first k rows of $\mathbf{A}$ have the same form as the corresponding rows in $\mathbf{H}$; after a relabelling of the tier 0 vertices (cf. (2.6)), the j-th row where $1 \le j \le k$ can be taken to be

$$[\,\mathbf{0}\ldots\mathbf{0}\ -\mathbf{1}\ +\mathbf{1}\ \mathbf{0}\ldots\mathbf{0}\,] \tag{4.6}$$

where the 3×3 diagonal matrices, $-\mathbf{1}, +\mathbf{1}$ are in columns $(2j-1)$ and $(2j)$ respectively. Note that the above relabelling is not used in the proof below.

The first k rows of $\mathbf{D}$ also have two non-zero entries, the j-th row is given by

$$\left[\frac{m_{2j-1}\,m_{2j}}{m_{2j-1}+m_{2j}}\right]\left(\mathbf{0}\ldots\mathbf{0}\,\frac{-\mathbf{1}}{m_{2j-1}}\ \ \frac{\mathbf{1}}{m_{2j}}\ \ \mathbf{0}\ldots\mathbf{0}\right) \tag{4.7}$$

(2) Next, row $j,\ k+1 \le j \le k+l$ of $\mathbf{H}$ has either 3 or 4 non-zero entries because it correspond to a tier 2 vertex of the tree. In the first case, $\chi_2(j)$ (4.2) (where j denotes the typical row as well as the corresponding virtual vertex, V_j) has one element, f in the set $\{2k+1,\ldots,N\}$ while $\chi_1(j)$ has 2 consecutive elements in the set $\{1,\ldots,2k\}$, which correspond exactly to those in $\chi(h)$ for some $h<j,\ \ 1\le h\le k$. The corresponding row in $\mathbf{A}$ is then given by

$$\left[\mathbf{0}\ldots\mathbf{0}\left(\frac{-m_{2k-1}}{m_{2k-1}+m_{2k}}\right)\ \left(\frac{-m_{2k}}{m_{2k-1}+m_{2k}}\right)\ \mathbf{0}\ldots\mathbf{0}\ \mathbf{1}\ \mathbf{0}\ldots\mathbf{0}\right] \tag{4.8a}$$

where the entry $\mathbf{1}$ is in column $f \in \chi_2(j)$

The same row in $\mathbf{D}$ is given by:

(4.8b)
$$\left[\frac{(m_{2h-1}+m_{2h})(m_f)}{m_{2h-1}+m_{2h}+m_f}\right]\ \left[\mathbf{0}\ldots\mathbf{0}\left(\frac{-\mathbf{1}}{m_{2k-1}+m_{2k}}\right)\ \left(\frac{-\mathbf{1}}{m_{2k-1}+m_{2k}}\right)\mathbf{0}\ldots\mathbf{0}\left(\frac{\mathbf{1}}{m_f}\right)\mathbf{0}\ldots\mathbf{0}\right]$$

In the second case, $\chi_1(j)$ and $\chi_2(j)$ both contain 2 elements from the set $\{1,\ldots,2k\}$; $\chi_1(j) = \chi(h)$ while $\chi_2(j)=\chi(i)$ where $1\le h<i\le k<j$. The corresponding rows in $\mathbf{A}$ and $\mathbf{D}$ are respectively,

(4.9a)
$$\left[\mathbf{0}\ldots\mathbf{0}\left(\frac{-m_{2k-1}}{m_{2k-1}+m_{2k}}\right)\ \left(\frac{-m_{2k}}{m_{2k-1}+m_{2k}}\right)\mathbf{0}\ldots\mathbf{0}\left(\frac{+m_{2i-1}}{m_{2i-1}+m_{2i}}\right)\ \left(\frac{+m_{2i}}{m_{2i-1}+m_{2i}}\right)\mathbf{0}\ldots\mathbf{0}\right]$$

(4.9b)
$$\left[\frac{(m_{2h-1}+m_{2h})(m_{2i-1}+m_{2i})}{m_{2h-1}+m_{2h}+m_{2i-1}+m_{2i}}\right]\times$$
$$\left[\mathbf{0}\ldots\mathbf{0}\left(\frac{-\mathbf{1}}{m_{2k-1}+m_{2k}}\right)\ \left(\frac{-\mathbf{1}}{m_{2k-1}+m_{2k}}\right)\mathbf{0}\ldots\mathbf{0}\left(\frac{+\mathbf{1}}{m_{2i-1}+m_{2i}}\right)\ \left(\frac{+\mathbf{1}}{m_{2i-1}+m_{2i}}\right)\mathbf{0}\ldots\mathbf{0}\right]$$

The above two paragraphs, (1) and (2) completely analyse the structure of the first k rows of $\mathbf{H}, \mathbf{A}$ and $\mathbf{D}$ (associated with the tier 1 vertices) and the next l rows of these matrices (associated with the tier 2 vertices). Equations (4.6) to (4.9) should provide sufficient motivation for the general formulae which shall be given next.

(3) As usual, the j-th row, $\mathbf{R}_j$, $1 \leq j \leq N-1$ is the typical row in $\mathbf{H}, \mathbf{A}$ and $\mathbf{D}$ belonging to a virtual vertex in any tier. Let the sets $\chi(j) = \chi_1(j) \cup \chi_2(j)$ be those defined in (4.2). Then the j-th row in $\mathbf{A}$ can be written in the form (where $R_j(i)$ is the i-th entry)

$$\mathbf{R}_j^A(n) = \begin{cases} -\dfrac{m_n}{\sum\limits_{h \in \chi_1(j)} m_h} & \text{if} \quad n \in \chi_1(j) \\ +\dfrac{m_n}{\sum\limits_{h \in \chi_2(j)} m_h} & \text{if} \quad n \in \chi_2(j) \\ \mathbf{0} & \text{if} \quad n \notin \chi(j). \end{cases} \tag{4.10a}$$

The j-th row in $\mathbf{D}$ takes the form:

$$\frac{\mathbf{R}_j^D(n)}{\left[\dfrac{\left(\sum\limits_{h \in \chi_1(j)} m_h\right)\left(\sum\limits_{h \in \chi_2(j)} m_h\right)}{\sum\limits_{h \in \chi(j)} m_h}\right]} = \begin{cases} \dfrac{-1}{\sum\limits_{h \in \chi_1(j)} m_h} & \text{if} \quad n \in \chi_1(j) \\ \dfrac{+1}{\sum\limits_{h \in \chi_2(j)} m_h} & \text{if} \quad n \in \chi_2(j) \\ 0 & \text{if} \quad n \notin \chi(j). \end{cases} \tag{4.10b}$$

All the links in the schema, (4.1) are in place and the proof of theorem 4.1 can now be given.

(4.1) Proof of Main Result. After the above preparation, it is now relatively straight forward to show that the symplectic condition, (7)

$$\mathbf{A}\ \mathbf{D}^t = \mathbf{I}_{3N}$$

holds for the matrices, $\mathbf{M}$, (5) which are derived from the spanning binary trees, $\mathbf{G}$ through schema (4.1).

Let $(\mathbf{R}_j, \mathbf{R}_h)$ be the inner product that takes into account the fact that each element of a row $\mathbf{R}_j$ is a 3×3 diagonal matrix (where all the diagonal elements are identical), that is,

$$(\mathbf{R}_j, \mathbf{R}_h) = \begin{bmatrix} (\mathbf{R}_j^{(1)}, \mathbf{R}_h^{(1)}) & & \\ & (\mathbf{R}_j^{(2)}, \mathbf{R}_h^{(2)}) & \\ & & (\mathbf{R}_j^{(3)}, \mathbf{R}_h^{(3)}) \end{bmatrix} \tag{4.11}$$

$\mathbf{R}_j^{(s)}, s = 1, 2, 3$ denotes the row consisting of the s-th diagonal elements; since all the diagonal elements are identical, the three nonzero diagonal entries in (4.11) are also identical. To prove (7), it will be sufficient to show that

$$(\mathbf{R}_j^A, \mathbf{R}_k^D) = \begin{bmatrix} \delta_{jk} & & \\ & \delta_{jk} & \\ & & \delta_{jk} \end{bmatrix}, \tag{4.12}$$

where the meaning of the superscripts A and D should be evident.

LEMMA 4.1. $(\mathbf{R}_j^A, \mathbf{R}_j^D) = \mathbf{I}_3$

Proof. From (4.10 a, b), it is clear that corresponding rows of $\mathbf{A}$ and $\mathbf{D}$ have entries of the same signs in identical columns. Thus

$$(\mathbf{R}_j^A, \mathbf{R}_j^D) = (\mathbf{R}_j^{A(1)}, \mathbf{R}_j^{d(1)})\mathbf{I}_3, \ 1 \le j \le N-1$$

where the scalar multiple in front of $\mathbf{I}_3$ is a positive number, given by

$$\sum_{n \in \chi_1(j)} \frac{m_n \left(\sum\limits_{h \in \chi_2(j)} m_h \right)}{\left(\sum\limits_{h \in \chi_1(j)} m_h \right) \left(\sum\limits_{h \in \chi(j)} m_h \right)} + \sum_{n \in \chi_2(j)} \frac{m_n \left(\sum\limits_{h \in \chi_1(j)} m_h \right)}{\left(\sum\limits_{h \in \chi_2(j)} m_h \right) \left(\sum\limits_{h \in \chi(j)} m_h \right)} \tag{4.13}$$

This number is one. For the N-th rows the inner product is easily seen to be also one. □

From the detailed construction of the matrices $\mathbf{A}$ and $\mathbf{D}$, one observes that the rows are grouped by tiers of the associated virtual vertices. For example, (4.6) and (4.7) describe the first k rows associated with the tier 1 vertices, (4.8 a, b) describe the next l rows associated with the tier 2 vertices and so on. The following result states that non-corresponding rows of $\mathbf{A}$ and $\mathbf{D}$ in each group, are *orthogonal*.

LEMMA 4.2. $(\mathbf{R}_j^A, \mathbf{R}_k^D) = \mathbf{0}$ *for* $\mathbf{V}_j, \mathbf{V}_k$ *in the same tier.*

Proof. The proof follows from the null intersection,

$$\chi(j) \cap \chi(k) = \emptyset, \tag{4.14}$$

because these sets locate the non-zero elements in $\mathbf{R}_j^A$ and $\mathbf{R}_k^D$. The null intersection (4.14) is a direct consequence of the fact that G is a tree that is, it does not have circuits. (cf. Lemma 2.1 where this is established from rule (i) for INTER). □

The next result extends Lemma 4.2 to the situations where the rows are not in the same group.

LEMMA 4.3. $(\mathbf{R}_j^A, \mathbf{R}_k^D) = \mathbf{0}$ *where the associated vertices* $\mathbf{V}_j, \mathbf{V}_k$ *are not in the same tier.*

Proof. There are two cases, namely

(i) $\mathbf{V}_j$ is connected to $\mathbf{V}_k$ (in a higher tier) by a path consisting only of vertices *lower* than $\mathbf{V}_k$.

(ii) $\mathbf{V}_j$ is *not* connected to $\mathbf{V}_k$ by such a path as in (i) (they may be connected by a path involving vertices higher than $\mathbf{V}_k$ in G).

In case (ii), $\chi(j)$ is not a subset of $\chi(k)$. In fact, $\chi(j) \cap \chi(k) = \emptyset$ because G is a tree. Therefore the result holds in this case.
In case (i), $\chi(j) \subset \chi(k)$ and there are two subcases, namely

(a) $\chi(j) \subset \chi_1(k)$ and,
(b) $\chi(j) \subset \chi_2(k)$.

A third alternative, that is,

$$\chi(j) \cap \chi_1(k) \neq \emptyset \quad \text{and,}$$
$$\chi(j) \cap \chi_2(k) \neq \emptyset$$

is impossible again because G is a tree (cf. Lemma 2.1), that is, it does not have *circuits*.
In subcase (a), the inner product reduces to

$$\sum_{n \in \chi_1(j)} \frac{-m_n \left(- \sum\limits_{h \in \chi_2(k)} m_h \right)}{\left(\sum\limits_{h \in \chi_1(j)} m_h \right) \left(\sum\limits_{h \in \chi(k)} m_h \right)} + \sum_{n \in \chi_2(j)} \frac{m_n \left(- \sum\limits_{h \in \chi_2(k)} m_n \right)}{\left(\sum\limits_{h \in \chi_2(j)} m_h \right) \left(\sum\limits_{h \in \chi(k)} m_h \right)} \tag{4.15}$$

The two terms cancel and (4.15) is zero. Subcase (b) is similar; the relevant entries in $\mathbf{R}_k^D$ are associated with $\chi_2(k)$ and therefore positive (cf. (4.3) for $\mathbf{H}$). The inner product reduces to the calculation,

$$\sum_{n \in \chi_1(j)} \frac{-m_n \left(\sum\limits_{h \in \chi_1(k)} m_h \right)}{\left(\sum\limits_{h \in \chi_1(j)} m_h \right) \left(\sum\limits_{h \in \chi(k)} m_h \right)} + \sum_{n \in \chi_2(j)} \frac{m_n \left(\sum\limits_{h \in \chi_1(k)} m_h \right)}{\left(\sum\limits_{n \in \chi_2(j)} m_h \right) \left(\sum\limits_{h \in \chi(k)} m_h \right)} \tag{4.16}$$

Again, the two terms in the above sum x cancels; the proof is complete. □

The same arguments work for the case when the rows are interchanged, that is, LEMMA 4.4. $(\mathbf{R}_k^A, \mathbf{R}_j^D) = \mathbf{0}$ *where the vertex* $\mathbf{V}_j$ *is lower than* $\mathbf{V}_k$.

LEMMA 4.5. $(\mathbf{R}_N^A, \mathbf{R}_j^D) = (\mathbf{R}_j^A, \mathbf{R}_N^D) = 0$ *for all* $j = 1, \ldots, N-1$.

Proof. The proof is trivial because all the entries in the N-th row of $\mathbf{A}$ and $\mathbf{D}$ have the same sign and it is easy to check that cancellation occurs in the above inner products.

Proof of Theorem 4.1. Lemmas 4.1 to 4.5 prove that (4.12) is valid for all the matrices generated by Schema (4.1) from spanning binary trees, G. Therefore, the symplectic condition, (7) has been verified and the proof of Theorem 4.1 complete.

V. Enumeration of trees and matrices. The total numbers of symplectic matrices, $\mathbf{M}$ generated by the above construction is calculated below.

THEOREM 5.1. *For a given N, the number of spanning binary trees with N leaves is*

$$\frac{(2N-3)!}{2^{N-2}}$$

Proof. A method due to Cayley (cf. [8]) for counting the number of spanning tree graphs in a complete graph, will be adopted for this calculation. To each tree, G which consists of $(2N-1)$ vertices, there belongs a word of length $(2N-3)$ over the alphabet $(1, 2, \ldots, N-1)$, that uniquely encodes G. The tree, G satisfies all the properties listed in Lemma 2.1, in particular properties $(c), (d)$ and (e). The vertices of G are ranked as follows: all the leaves, $\{\mathbf{q}_j\}_{j=1}^{N}$ are ranked by the subscript j, all the virtual vertices are again ranked by the subscript j, and all the leaves rank lower than the virtual vertices, $\{\mathbf{V}_j\}_{j=1}^{N-1}$.

In choosing the first element in the word for G, remove the leave which has the lowest rank, i.e. $\mathbf{q}_1$. The first element is then the subscript of the vertex in G which was adjacent to the removed vertex. In this process, the original tree G is cut down from the leaves; as a result, some of the original vertices of degrees greater than one, are subsequently reduced to vertices of degree one. Continuing this process, the i-th element in the word for G is determined by removing the vertex of current degree one, which has the lowest rank; the i-th element is then the subscript of the vertex which was adjacent to the removed one. The process stops when only two vertices remain. For example, the tree $G_2^2(5)$ in figure 1c, has the name-word, $\{1\ 1\ 2\ 2\ 4\ 3\ 3\}$. Note that no vertex, originally of degree one in G, appears in the word. This explains the reason for the alphabet $(1, 2, \ldots, N-1)$ which are just the subscripts of the vertices with degrees ≥ 2. The converse of the above process is also true, that is, one can construct a unique tree G with $(2N-1)$ vertices and N leaves from a word of length $(2N-3)$ over the alphabet $(1, \ldots, N-1)$ (cf. [8], page 49, 50).

Thus there is a one-to-one correspondence between the trees, G and words of length $(2N-3)$ over the alphabet, $(1, 2, \ldots, N-1)$, Because the virtual vertices of G, with the exception of the root, $\mathbf{V}_{N-1}$, have degree 3, the alphabet $(1, 2, \ldots, N-2)$ will appear *exactly twice* in its name-word, while the number $(N-1)$ will appear only *once*. Therefore, there are

$$\begin{array}{ll} (2N-3) & \text{ways to put } (N-1) \\ \dfrac{(2N-4)(2N-5)}{2} & \text{ways to put } 1 \\ \cdots\cdots & \\ \dfrac{(2)\,(1)}{2} & \text{ways to put } (N-2) \end{array}$$

in the word of length $(2N-3)$. This completes the proof. □

The number of $(6N \times 6N)$ symplectic matrices generated by schema (4.1) or equivalently (3.4), (3.5) and (3.6), from the spanning binary trees, G with N leaves, is calculated in the corollary below.

COROLLARY 5.1. *For a given N, there are $4(2N-3)!$ $(6N \times 6N)$ symplectic matrices, constructed from the trees, G.*

Proof. The proof is based on the observation that for each undirected tree, G with N leaves, there are $(2)^N$ ways to generate the symplectic matrices, $\mathbf{M}$ via (4.1). This is because for each virtual vertex, $\mathbf{V}_j$ in G, there are 2 ways to choose the arguments of INTER, ARG $1(j)$ and ARG $2(j)$. In other words, the binary operation INTER is *symmetric* in its arguments. Equivalently, the sets $\chi_1(j)$ and $\chi_2(j)$ defined in (4.2) can be interchanged (or the 2 branches descending from the vertex, $\mathbf{V}_j$ can be interchanged). Finally, the sign of the N-th row of $\mathbf{A}$ can be either positive or negative.

Theorem 5.1 implies that there are $(2^N)\dfrac{(2N-3)!}{2^{N-2}}$ such symplectic matrices. □

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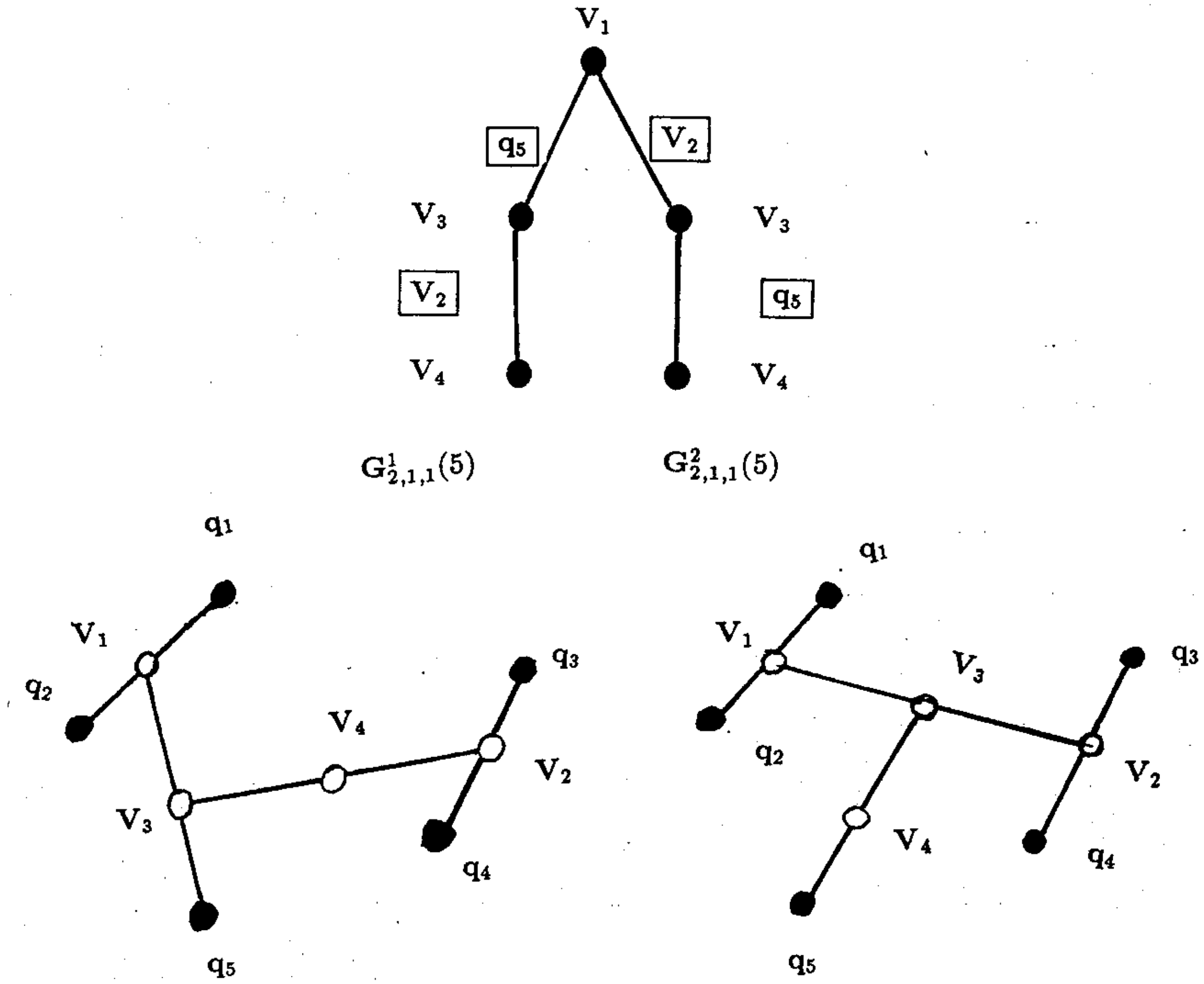
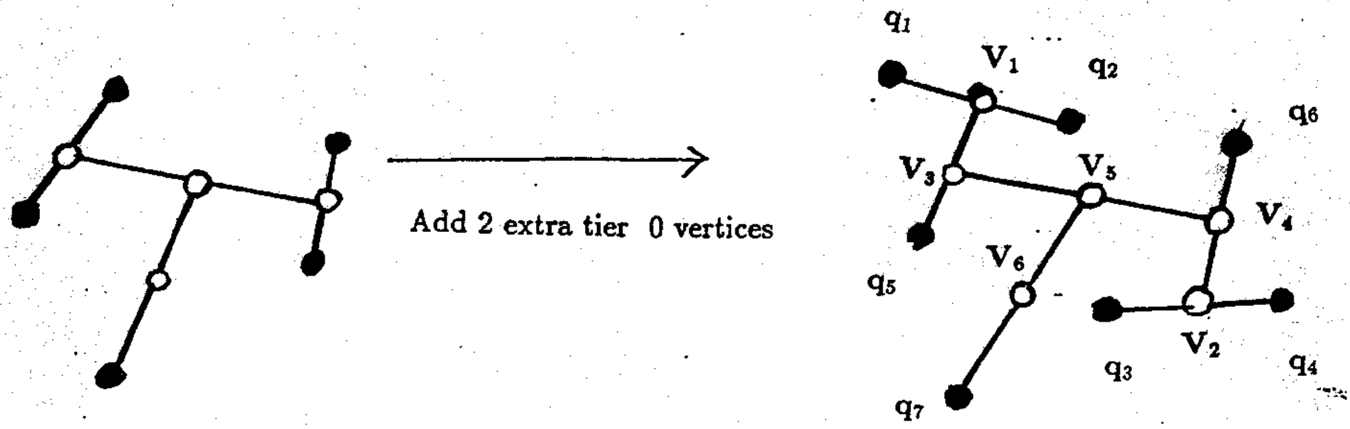
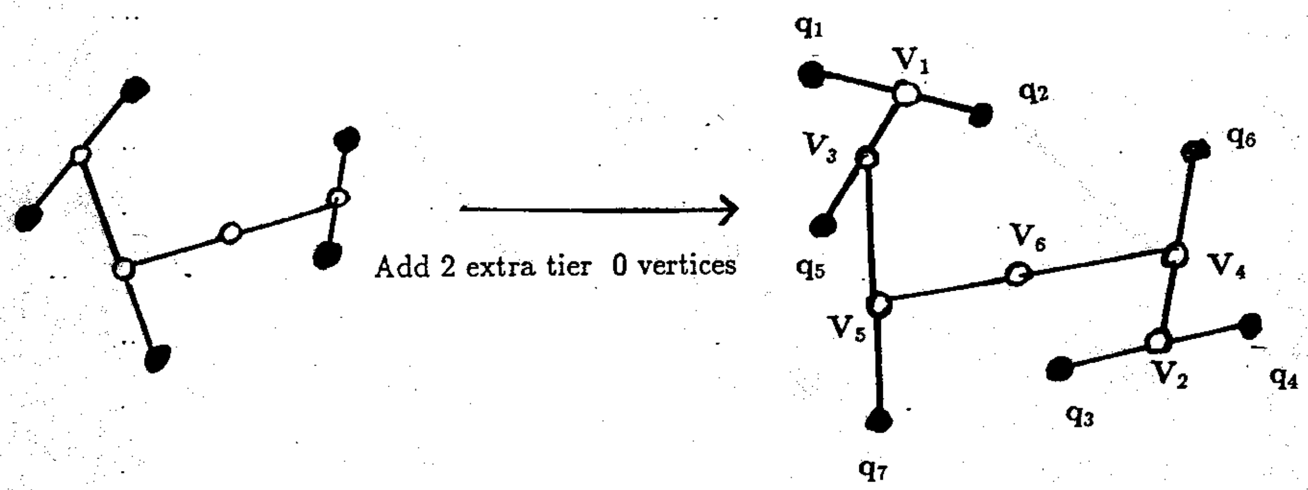


Figure 1: (a) Associated tree, A_5^2
(b), (c) Spanning tree graphs, $G^s_{2,1,1}(5)$, $s = 1, 2$



$G_2^2(5)$

$H^2_{2,2,1,1}(7)$



$G_2^1(5)$

$H^1_{2,2,1,1}(7)$

Figure 2: Symplectic Tree Graphs generated by A_N^k indirectly. From $G^s_{2,1,1}(5)$, $s = 1, 2$, the corresponding $H^s_{2,2,1,1}(7)$ are generated by adding 2 vertices, keeping $k = 2$ constant but increasing the # of tier 2 virtual vertices to $l = 2$. In both examples, the tier 1 vertices are V_1, V_2 and the tier 2 vertices are V_3, V_4.