ON SYMPLECTIC TREE GRAPHS

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Abstract. A new method for generating canonical transformations of first-order hamiltonian systems is discussed. The method is graph-theoretical and provides a useful classification of some symplectic matrices. Beginning with a complete graph, $\mathbf{K}_N$ associated with N-body Hamiltonians, a class of spanning tree graphs, consisting of $2N-1$ vertices is generated by a well-defined procedure. Each tree graph in this class encodes a linear canonical transformation. A graph-theoretic device is used to enumerate these tree graphs (symplectic trees) and for given N, there are $\frac{(2N-3)!}{2^{N-2}}$ equivalence classes of canonical transformations of this type.

I. Introduction. In this paper, we describe a new class of symplectic transformations for Hamiltonians having the complex form†

$$H(z_1, \ldots, z_N) = \sum_{j,k=1}^{N}{}' \Gamma_j \Gamma_k F_{jk}(z_j - z_k) \tag{1.1}$$

where (a) Γ_j are real constants, (b) F_{jk} are analytic functions of one complex variable except possibly at a finite number of isolated singularities, (c) the argument of F_{jk} are the vector differences $z_j - z_k$ where $z_j \in \mathbb{C}$. The complex equations of motion for (1.1) are

$$\Gamma_j \dot{\bar{z}}_j = i \frac{\partial H}{\partial z_j} \quad , \quad j = 1, \ldots, N. \tag{1.2}$$

This complex formulation has a simple relationship with the standard (real) Hamiltonian formulation:

$$H_R(p_1, \ldots, p_N;\ q_1 \ldots, q_N) = Re\{H(z_1, \ldots, z_N)\}. \tag{1.3a}$$

$$\dot{q}_j = \text{sign}(\Gamma_j) \frac{\partial H_R}{\partial p_j} \quad , \quad \dot{p}_j = -\text{sign}(\Gamma_j) \frac{\partial H_R}{\partial q_j} \quad , \quad j = 1, \ldots, N \tag{1.3b}$$

where

$$q_j = \sqrt{|\Gamma_j|} x_j \quad , \quad p_j = \sqrt{|\Gamma_j|}\, y_j\ . \tag{1.4}$$

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†The Hamiltonian (1.1) is chosen for the sake of providing a concrete example for the reader. More general forms of first-order hamiltonians can be treated by our method (cf. section V)

and the signatures in (1.3b) depend on the sign of the "weights" Γ_j. Henceforth, we will discuss only the case where $\Gamma_j > 0$; the case of mixed signs differs only in minor details. Putting the real and imaginary parts together, i.e.

$$w_j = q_j + ip_j = \sqrt{\Gamma_j}\, z_j \tag{1.5}$$

we obtain the complex Hamiltonian formulation

$$\dot{\overline{\omega}}_j = i\,\frac{\partial \mathbf{H}}{\partial \omega_j}, \qquad \dot{\omega}_j = -i\frac{\partial \mathbf{H}}{\partial \overline{\omega}_j} \tag{1.6}$$

where the Hamiltonian, H (1.1) written in the form

$$\begin{aligned} \mathbf{H}(\omega_j, \overline{\omega}_j) &= \frac{1}{2}\left\{H(\omega_j) + H(\overline{\omega}_j)\right\} \\ &= \frac{1}{2}\left\{H(\omega_j; j = 1, \ldots, N) + C.C.\right\}. \end{aligned} \tag{1.7}$$

is taken to be a function of $2N$ independent complex variables.

By interpreting the complex variables, z_j as locations of N particles and the real quantities Γ_j as "weights" associated with these particles, the above family of Hamiltonians represent first–order N-body Problems with pairwise interactions. The term *first-order* refers to the property that these Hamiltonian systems do not originate from Newton's equations of motion (there is no acceleration and thus no second order time derivatives). Instead of conjugate momenta, the conjugate variables are position quantities, (1.4). A good example is vortex dynamics [1, 2] where the Hamiltonians arise from a velocity potential. Other examples of first-order N-body problems can be found in mathematical biology [3] and plasma physics [4].

The symplectic transformations we are concerned with, reduce the Hamiltonians (1.1) by one degree of freedom through their inherent translational symmetry. Historically, these transformations can be compared with the Jacobi coordinates in Celestial Mechanics [5] where the Hamiltonians are second-order because they essentially embody Newton's equations of motion. These new symplectic transformations turn out to be useful for treating a large class of Hamiltonian systems as *nearly integrable* problems, which extends the methods discussed in Lim [6, 7, 8, 9].

II. Tree Graphs. To every pair of positive integers $(j \neq k)$ $j, k \leq N$, there belongs a term in the Hamiltonian, (1.1); thus we can abstractly represent (1.1) by a *complete graph*, $\mathbf{K}_n$ with N vertices, $\{z_j\}$. A graph is *complete* if every pair of vertices define an *edge* (cf. [10]). Our results can now be stated concisely in graph-theoretic terms.

We will give a procedure for generating spanning tree graphs, $\mathbf{G}_k^s(\mathbf{N})$, consisting of N original vertices from $\mathbf{K}_N$ and $(N-1)$ virtual vertices. Since there are many *admissible* spanning tree-graphs for a given complete graph, K_N, we code these alternatives in terms of the branches of an associated tree, $\mathbf{A}_N^k$. Each branch of $\mathbf{A}_N^k$ represent a tree graph, $\mathbf{G}_K^s(N)$ that is associated with an equivalence class of symplectic transformations for (1.1). Thus we have the following scheme:

$$\begin{array}{ccc} \{\omega_j\}_{j=1}^{N} & \xrightarrow{\mathbf{T}_k^s(N)} & \{\rho_\alpha\}_{\alpha=1}^{N} \\ \big\downarrow & & \big\uparrow (C) \\ K_N & \xrightarrow{A_N^k} & G_k^s(N) \end{array} \tag{2.1}$$

where $\{\rho_a\}$ are the new coordinates given by the matrix $\mathbf{T}_k^s(N)$ in terms of the original coordinates $\{\omega_j = \sqrt{|\Gamma_j|}\ z_j\}$. The *leg*, $(\mathbf{C})$ represents formulae, (4.4) and (4.5) that generates $\{\rho_\alpha\}_{\alpha=1}^{N}$ from the $N-1$ virtual vertices of $G_k^s(N)$.

The details of this scheme will be given in the following sections. The main results will be stated and proofs given in sections IV and V. In summary, Theorem 4.1 states that for every positive integers $N \geq 2$ and "admissible" positive integers k, s the matrix $\mathbf{T}_k^s(N)$ in schema (2.1) generates symplectic transformations. Lemma 5.1 gives properties of the spanning tree graphs $\mathbf{G}_k^s(N)$ and Theorem 5.1 counts the number of symplectic transformations (for fixed N)

III Associated Trees. First we describe the basic binary operation that underlies our procedure for generating the virtual vertices in $\mathbf{G}_k^s(N)$. This operation called INTER is given by

$$\begin{aligned} V &= INTER(A, B) \\ &= \frac{\Gamma(A)A + \Gamma(B)\ B}{\Gamma(A) + \Gamma(B)}; \quad V, A, B \in \mathbb{C} \end{aligned} \tag{3.1}$$

where $V = V_j$ is a new virtual vertex while the arguments A, B can be either a virtual vertex that has already been generated, i.e. V_h for some $h < j$ or one of the original vertices in $\mathbf{K}_N$, z_q. To complete the production of a virtual vertex, its weight is calculated as follows:

$$\Gamma(V) = \Gamma(A) + \Gamma(B). \tag{3.2}$$

The above averaging operation is governed by two rules:

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

(ii) to *begin*, $k \leq [N/2]$ non-adjacent edges in $\mathbf{K}_N$ are preselected to produce the first k virtual vertices, $\mathbf{V}_j$ $1 \leq j \leq k$ in tier 1 (in this convention, z_q are in tier 0).

After a relabelling (if necessary) of the original vertices, $\{z_j\}$, the first (tier 1) virtual vertices are:

$$
\begin{aligned}
\mathbf{V}_1 &= INTER\ (z_1, z_2) \\
\mathbf{V}_2 &= INTER\ (z_3, z_4) \\
&\vdots \\
\mathbf{V}_k &= INTER\ (z_{2k-1},\ z_{2k})
\end{aligned}
\tag{3.3}
$$

The number of tier 1 virtual vertices is assigned to the index k in the labels $\mathbf{G}_k^s(N)$ as well as $\mathbf{A}_N^k$.

For N large compared to k, there are clearly many possible ways to generate the virtual vertices in $\mathbf{G}_k^s(N)$. In order to make sense of this complexity and to describe the variety involved, we introduce an associated tree $\mathbf{A}_N^k$ for each N and each $k \leq [N/2]$. The *branches* of $\mathbf{A}_N^k$ codify the different ways of constructing the tree-graphs $\mathbf{G}_k^s(N)$ from the complete graph, $\mathbf{K}_N$. The superscript s in the label $\mathbf{G}_k^s(N)$ denotes the branch of $\mathbf{A}_N^k$ associated with the spanning tree-graph. This will become clearer when we construct examples of the associated trees.

We begin with the example $\mathbf{A}_5^2$ (cf. fig. 1). In this case $k = 2$ is the maximum number of tier 1 virtual vertices allowed for the complete graph $\mathbf{K}_5$. They are

$$
\begin{aligned}
\mathbf{V}_1 &= INTER(z_1, z_2) \\
\mathbf{V}_2 &= INTER(z_3, z_4).
\end{aligned}
\tag{3.4}
$$

The root of $\mathbf{A}_5^2$ is denoted by $\mathbf{V}_1$. From the root there are two distinct ways to generate the vertex $\mathbf{V}_3$. On the right branch, $\mathbf{V}_3 = INTER(\mathbf{V}_1, \mathbf{V}_2)$ on the left, $\mathbf{V}_3 = INTER(\mathbf{V}_1, z_5)$. We see this clearly in the tree graphs $\mathbf{G}_2^2(5)$ where $s = 1, 2$ for the left and right branches respectively (see fig 1.b,c). Moving down the branches of $\mathbf{A}_5^2$, $\mathbf{V}_4 = INTER(\mathbf{V}_3, z_5)$ on the right and $\mathbf{V}_4 = INTER(\mathbf{V}_3, \mathbf{V}_2)$ on the left. There are no more branching in the associated tree. The two branches of $\mathbf{A}_5^2$ have the path representations

$$
\begin{aligned}
\mathbf{G}_2^2(5) &= \left\{ \boxed{\mathbf{V}_2},\ \boxed{z_5} \right\} \\
\mathbf{G}_2^1(5) &= \left\{ \boxed{z_5},\ \boxed{\mathbf{V}_2} \right\}
\end{aligned}
\tag{3.5}
$$

where the boxed quantities denote the edges of $\mathbf{A}_5^2$ to distinguished them from the vertices, after which they were named.

It is now easy to specify the properties of the general associated tree, $\mathbf{A}_N^k$:

(i) the root is always labelled $\mathbf{V}_1$,

(ii) the branches code the generation of the virtual vertices in tiers ≥ 2; beginning with $\mathbf{V}_{k+1}$ and ending with $\mathbf{V}_{N-1}$, the vertices of $\mathbf{A}_N^k$ below the root appear in the same order (increasing subscript) on each branch; it is assumed that the tier 1 vertices, $\mathbf{V}_j, j = 1, \dots, k$, are generated according to (3.3).

(iii) the edges of $\mathbf{A}_N^k$ are labelled by boxed vertices consisting of *only* the z_j, $2k+1 \leq j \leq N$, and the tier 1 vertices, $\mathbf{V}_j$, $j = 1, \dots, k$.

(iv) an edge, $\boxed{v} = (u, \omega)$, where ω is the lower vertex, encodes the operation $\omega = INTER(u, v)$.

Additional properties of the *canonical* associated tree are:

(v) the tier 1 vertices, $\mathbf{V}_j$, $j = 1, \dots, k$, appear in the path representation of the branches of $\mathbf{A}_N^k$ (the canonical associated tree is denoted by the same label), in the order of increasing j.

(vi) the same holds for the order in which $z_j, z_k + 1 \leq j \leq N$, appear in the path-representations.

In graph-theoretic terms [10] an edge in $\mathbf{A}_N^k$ is given by an ordered pair of vertices, e.g.

$$\boxed{z_q} = (\mathbf{V}_j,\ \mathbf{V}_l), \qquad l > j \tag{3.6}$$

which represents the INTER operation,

$$\mathbf{V}_l = INTER(\mathbf{V}_j,\ z_q). \tag{3.7}$$

The vertex z_q after which the edge is named, appears as the second argument in (3.7). Property (iii) states that only the original vertices z_q, $2k+1 \leq q \leq N$ and k tier 1 virtual vertices are used as second arguments in INTER. Properties (i) and (ii) for the vertices of $\mathbf{A}_N^k$ states that all the higher tiered virtual vertices, $\mathbf{V}_j, k+1 \leq j \leq N-1$ are generated consecutively in $\mathbf{G}_k^s(N)$. In other words there is only one virtual vertex in each tier above tier 1. It is obvious that the virtual vertices in all the branches of A_N^k that are in the same tier appear at the same level in the tree In section 5, we will comment on spanning tree graphs that are not generated by the associated tree $\mathbf{A}_N^k$, e.g. those with more than one tier 2 virtual vertices.

Properties (v) and (vi) of the canonical tree specify the *canonical* order in which the tier 1 virtual vertices and the original vertices (tier 0) separately enter as second arguments in INTER. Clearly, a different order is equivalent to a relabelling of the original vertices of $\mathbf{K}_N$ by a permutation on N integers. Two spanning tree graphs generated by the same branch of $\mathbf{A}_N^k$ but differing by such a permutation are said to be *equivalent*. Thus the branches of the canonical $\mathbf{A}_N^k$, i.e. $\mathbf{G}_k^s(N)$ represent *not* only one spanning tree graph with $2N-1$ vertices but also an equivalence class of these.

On the other hand, it is important to note that the *order* in which a tier 1 virtual vertex appears *vis-a-vis* a tier 0 original vertex in the path representation of a branch completely defines the equivalence class. For example the path representations (3.5) for $\mathbf{A}_5^2$ can be given in binary:

$$\mathbf{G}_2^2(5) = \{1\ 0\} \qquad (3.8)$$
$$\mathbf{G}_2^1(5) = \{0\ 1\}$$

where a 0 denotes a tier 0 original vertex, eg. z_5 and a 1 denotes a tier 1 virtual vertex, e.g. $\mathbf{V}_2$. This gives a convenient algorithm to count the number of branches (equivalence classes of spanning three graphs) in $\mathbf{A}_N^k$. Since only

$$\begin{array}{rl} (N-2k) & \text{tier 0 vertices and,} \\ (k-1) & \text{tier 1 vertices} \end{array} \qquad (3.9)$$

can appear in the path representations by property (iii) of $\mathbf{A}_N^k$, we have the following result

THEOREM 3.1. *There are* $\binom{N-k-1}{k-1}$ *branches in* $\mathbf{A}_N^k$.

Now we can properly define the significance of the index s in the label $\mathbf{G}_k^s(N)$. It takes the value of the binary number obtained when the path representation of $\mathbf{G}_k^s(N)$ is put in binary form. For example, (3.8) assigns the values $s = 1, 2$ to the left and right branches respectively of $\mathbf{A}_5^2$ We note that the value of the index, s, is a characteristic of the equivalence class, $\mathbf{G}_k^s(N)$, uniquely defined by its binary representation.

In summary, we observe that the canonical associated tree, $\mathbf{A}_N^k$ can be completely and uniquely represented by a sequence of binary numbers which consist of $(N-k-1)$ digits. For example, $\mathbf{A}_7^3$ is given by the binary numbers in increasing order

$$\begin{aligned} \mathbf{G}_3^3(7) &= \{0\ 1\ 1\} \\ \mathbf{G}_3^5(7) &= \{1\ 0\ 1\} \qquad (3.10) \\ \mathbf{G}_3^6(7) &= \{1\ 1\ 0\} \end{aligned}$$

Figure 2 depicts the canonical tree, $\mathbf{A}_7^3$, which clearly shows that the labels for its edges and vertices can be read off from (3.10), because of the separate *canonical* order of appearance of the tier 0 edges, $\boxed{z_q}$, and the tier 1 edges, $\boxed{\mathbf{V}_j}$; the vertices of $\mathbf{A}_7^3$ below the root, always appear in order from $\mathbf{V}_4$ to $\mathbf{V}_6$. Anticipating section IV we note that the proof of the main result, theorem 4.1, depends *only* on the binary representation of a spanning tree, $\mathbf{G}_k^s(N)$ and *not* its individual characteristics.

IV Symplectic Transformations. For each spanning tree graph, $\mathbf{G}_k^s(N)$, constructed according to the corresponding branch on the associated tree $\mathbf{A}_N^k$, from the complete graph, $\mathbf{K}_n$, there belongs a linear transformation acting on $\mathbb{C}$ given by the following given by the following procedure. Let

$$\begin{aligned} ARG1(q) &= \text{1st argument in INTER that generated } \mathbf{V}_q, \\ &\qquad \text{the } q\text{-th virtual vertex.} \\ ARG2(q) &= \text{2nd argument in the same binary operation.} \end{aligned} \tag{4.1}$$

In other words,

$$\mathbf{V}_q = INTER\,(ARG1(q), ARG2(q)) \tag{4.2}$$

and the weight of $\mathbf{V}_q$ is

$$\Gamma(\mathbf{V}_q) = \Gamma(ARG1(q)) + \Gamma(ARG2(q)). \tag{4.3}$$

Then for every virtual vertex $\mathbf{V}_q$ in the graph $\mathbf{G}_k^s(N)$, we define

$$\rho_q = \left[\frac{\Gamma(ARG1(q)) \cdot \Gamma(ARG2(q))}{\Gamma(ARG1(q)) + \Gamma(ARG2(q))}\right]^{\frac{1}{2}} (ARG2(q) - ARG1(q)) \tag{4.4}$$

for $q = 1, \ldots, N-1$. Completing this with

$$\rho_N = \frac{\left(\sum_{j=1}^N \Gamma_j\ z_j\right)}{\sum_{j=1}^N \Gamma_j}, \tag{4.5}$$

we obtain a (real) linear transformation on $\mathbb{C}^N$.

From the above transformation given in terms of the tier 0 vertices z_j of the complete graph k_N, we derive a transformation $\mathbf{T}_k^s : \mathbb{R}^{2N} \longrightarrow \mathbb{R}^{2N}$ defined in terms of the original symplectic coordinates, (1.5) for the Hamiltonian (1.1). Since the original (complex) symplectic coordinates (1.5) are obtained simply by multiplying each vertex of k_N by the square-root of its weight, i.e.

$$\omega_j = \sqrt{\Gamma_j}\ z_j \quad , \quad j = 1, \ldots, N \tag{4.6}$$

we get the desired transformation $\mathbf{T}_k^s(N)$ (in terms of the real and imaginary parts of ω_j) by substituting $\omega_j/\sqrt{\Gamma_j}$ for z_j in (4.4) and (4.5) and taking real and imaginary parts. We postpone the proof of the main result that the transformation $\mathbf{T}_k^s(N)$ is *symplectic* for every $\mathbf{G}_k^s(N)$ in $\mathbf{A}_k^N$. First we provide an example $\mathbf{T}_2^2 : \mathbb{C}^5 \longrightarrow \mathbb{C}^5$ class of symplectic transformations. From the spanning tree graph $G_2^2(5)$ (cf. figure 1c), we obtain via (4.4), (4.5) and (4.6) the transformation $T_2^2(5)$:

$$
\begin{aligned}
(4.7) \qquad \rho_1 &= \left[\frac{\Gamma_1\Gamma_2}{\Gamma_1+\Gamma_2}\right]^{1/2}\left(\frac{\omega_2}{\sqrt{\Gamma_2}}-\frac{\omega_1}{\sqrt{\Gamma_1}}\right)\\
\rho_2 &= \left[\frac{\Gamma_3\Gamma_4}{\Gamma_3+\Gamma_4}\right]^{1/2}\left(\frac{\omega_4}{\sqrt{\Gamma_4}}-\frac{\omega_3}{\sqrt{\Gamma_3}}\right)\\
\rho_3 &= \left[\frac{(\Gamma_1+\Gamma_2)(\Gamma_3+\Gamma_4)}{\Gamma_1+\Gamma_2+\Gamma_3+\Gamma_4}\right]^{1/2}\left(\frac{\sqrt{\Gamma_4}\omega_4+\sqrt{\Gamma_3}\omega_3}{\Gamma_3+\Gamma_4}-\frac{\Gamma_1\omega_1+\sqrt{\Gamma_2}\omega_2}{\Gamma_1+\Gamma_2}\right)\\
\rho_4 &= \left[\frac{(\Gamma_1+\Gamma_2)(\Gamma_3+\Gamma_4)(\Gamma_5)}{\sum\limits_{i=1}^{5}\Gamma_i}\right]^{1/2}\left(\frac{\omega_5}{\sqrt{\Gamma_5}}-\frac{\sum_{i=1}^{4}\sqrt{\Gamma_i}\omega_i}{\sum\limits_{i=1}^{4}\Gamma_i}\right)\\
\rho_5 &= \frac{\sum\limits_{i=1}^{5}\sqrt{\Gamma_i}\omega_i}{\sum\limits_{i=1}^{5}\Gamma_i}
\end{aligned}
$$

Taking the real and imaginary parts of (4.7) to obtain the usual (real) canonically conjugate variables, it can be verified directly that the Jacobian matrix, $\mathbf{M}$ of $\mathbf{T}_2^2(5)$ (viewed as a linear transformation from $\mathsf{R}^{10} \longrightarrow \mathsf{R}^{10}$) is a *symplectic* matrix, i.e. $\mathbf{M}^t\mathbf{J}\mathbf{M} = \mathbf{J}$. Thus $\mathbf{T}_2^2(5)$ (4.7) is a *symplectic* transformation and it provides a realization of the schema, (2.5):

$$
(4.8) \qquad
\begin{array}{ccc}
\{\omega_j\}_{j=1}^{5} & \xrightarrow{\quad \mathbf{T}_2^2(5) \quad} & \{\rho_j\}_{j=1}^{5} \\
\big\downarrow & & \big\uparrow (C) \\
K_5 & \xrightarrow{\quad A_5^2 \quad} & G_2^2(5)
\end{array}
$$

where (C) is given by (4.4), (4.5). The quantity $\rho_5 \in \mathbb{C}$ in this example, (4.7) (ρ_N (4.5) in general) represents the "average" position of the ensemble of $5(N)$ particles. Since it does not appear explicitly in the transformed Hamiltonian, we conclude that its real and imaginary parts are necessarily *invariant*. Therefore the symplectic transformations $\mathbf{T}_k^s(N)$ generate a reduction by one degree of freedom which is essentially due to the translational symmetry of the Hamiltonians (1.1).

THEOREM 4.1. *For every spanning tree graph,* $\mathbf{G}_k^s(N)$ *on the canonical associated trees* $\mathbf{A}_N^k$ *where* $k \le \left[\frac{N}{2}\right]$*, there belongs a symplectic transformation* $\mathbf{T}_k^s(N) : \mathbb{R}^{2N} \longrightarrow \mathbb{R}^{2N}$.

A relabelling of the tier 0 vertices by permutations on N integers gives an equivalence relation on the graphs $\mathbf{G}_k^s(N)$ so that to each branch of the associated trees A_N^k there actually belongs an equivalence class of spanning tree graphs, again denoted by $\mathbf{G}_k^s(N)$ (note the minor abuse in notation). This implies the corollary:

COROLLARY 4.1. *Each spanning tree graph in the equivalence class (modulo above relabelling)* $\mathbf{G}_k^s(N)$ *generates a linear symplectic transformation* $\mathbf{T}_k^s(N) : \mathbb{R}^{2N} \longrightarrow \mathbb{R}^{2N}$.

We will also denote the equivalence class of symplectic transformation by $\mathbf{T}_k^s(N)$

To prove Theorem 4.1, we make some observations about the class of transformations generated by taking real and imaginary parts of (4.4), (4.5) and (4.6).:

(i) $\mathbf{T}_k^s(N) : \mathbb{R}^{2N} \longrightarrow \mathbb{R}^{2N}$ is linear and real,

(ii) it is given by the matrix $\mathbf{M}$, i.e.

$$\underset{\sim}{\rho} = \mathbf{M}\underset{\sim}{\omega} \quad \text{where}$$

$$\underset{\sim}{\rho} = \left[\rho_1^r, \ldots, \rho_N^r, \rho_1^i, \ldots, \rho_N^i\right]^t \tag{4.9}$$

$$\underset{\sim}{\omega} = \left[\omega_1^r, \ldots, \omega_N^r, \omega_1^i, \ldots, \omega_N^i\right]^t$$

(the superscript r, i denote real and imaginary parts)

$$\mathbf{M} = \begin{bmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{A} \end{bmatrix} \text{where } \mathbf{A} \text{ is a real } N \times N \text{ matrix.}$$

(iii) linearity implies that the Jacobian matrix of $\mathbf{T}_k^s(N)$ is again given by $\mathbf{M}$.

(iv) by definition, $\mathbf{T}_k^s(N)$ is a *symplectic* transformation *iff* its Jacobian matrix $\mathbf{M}$ is *symplectic* i.e.

$$\mathbf{M}^t\mathbf{J}\,\mathbf{M} = \mathbf{J} \qquad \text{where} \tag{4.11}$$

$$\mathbf{J} = \begin{bmatrix} 0 & \mathbf{I}_N \\ -\mathbf{I}_N & 0 \end{bmatrix};$$

(ii) and (iii) imply that $\mathbf{M}$ is *symplectic iff*

$$\mathbf{A}^t\mathbf{A} = \mathbf{I}_N \quad , \quad \text{that is } \mathbf{A} \text{ is } \textit{orthogonal.} \tag{4.12}$$

The matrix $\mathbf{A}$ will be given explicitly here, thus providing more details of the transformation $\mathbf{T}_k^s(N) : \mathbf{C}^N \longrightarrow \mathbf{C}^N$ which is already described algorithmically in (4.4), (4.5) and (4.6):

(a) the first k rows of $\mathbf{A}$ are generated by the k tier 1 vertices and a typical row (say j-th row) is given by

$$\mathbf{C}_j \left[0\ldots0 \quad \frac{-1}{\sqrt{\Gamma_{2j-1}}} \quad \frac{1}{\sqrt{\Gamma_{2j}}} \quad 0\ldots0\right] \tag{4.13}$$

where the only non-zero entries are in columns $(2j-1)$ and $(2j)$ and the constant $\mathbf{C}_j$ is given by

$$\mathbf{C}_j = \left[\frac{\Gamma_{2j-1}\,\Gamma_{2j}}{\Gamma_{2j-1}+\Gamma_{2j}}\right]^{1/2} \tag{4.14}$$

(b) next, rows $k+1)$ to $(N-1)$ are generated consecutively by the virtual vertices in tiers ≥ 2 (there is only one vertex in each of the higher tiers): the typical q-th row say is given by two possibilities, depending on whether the second argument $ARG2(q)$ is a tier 0 vertex (i.e. z_j , $2k+1 \leq j \leq N$) or a tier 1 vertex (i.e. $\mathbf{V}_j$, $2 \leq j \leq k$) which is uniquely specified in the binary path representation of $\mathbf{G}_k^s(N)$ in the canonical associated tree $\mathbf{A}_k^N$. The only non-zero entries in the q-th row are

(4.15a)

$$-\mathbf{C}_q\left(\frac{\sqrt{\Gamma_m}}{\sum\limits_{p\in\chi_{q-1}}\Gamma_p}\right)$$

is the m-th entry for each $m \in \chi_{q-1}$ in both cases,

$$\begin{cases} \mathbf{C}_q\left(\dfrac{1}{\sqrt{\Gamma_j}}\right) \text{ is the } j\text{-th entry in the first case} \\ \text{where } j \text{ is the subscript of } ARG2(q). \\ \dfrac{\mathbf{C}_q}{\Gamma_{2j-1}+\Gamma_{2j}}\left[\sqrt{\Gamma_{2j-1}} \quad \sqrt{\Gamma_{2j}}\right] \text{ are the } (2j-1) \\ \text{and } (2j)\text{-th entries in the second case.} \\ \text{where } j \text{ is the subscript of } ARG2(q) \end{cases}$$

$$\mathbf{C}_q = \left[\frac{\left(\sum\limits_{p\in\chi_{q-1}}\Gamma_p\right)\begin{cases}(\Gamma_j) & \text{in the first case}\\ (\Gamma_{2j-1}+\Gamma_{2j}) & \text{in the second case}\end{cases}}{\sum\limits_{p\in\chi_q}\Gamma_p}\right]^{1/2} \tag{4.15b}$$

where χ_{q-1} is the subset of integers $p \in \{1, \ldots, N\}$ such that the tier 0 vertex z_p enters into the definition of the $(q-1)$-th virtual vertex, i.e.

$$(4.16) \qquad \begin{aligned} ARG1(q) = V_{(q-1)} &= \frac{\sum_{p \in \chi_{q-1}} \Gamma_p \, z_p}{\sum_{p \in \chi_{q-1}} \Gamma_p} \\ &= \frac{\sum_{p \in \chi_{q-1}} \sqrt{\Gamma_p} \, \omega_p}{\sum_{p \in \chi_{q-1}} \Gamma_p} \qquad \text{for } k+2 \le q \le N-1 \end{aligned}$$

(for $q = k+1$, $\mathbf{V}_{(q-1)}$ is taken to be $\mathbf{V}_1$). This is a good place to remark that the virtual vertex $\mathbf{V}_q$, $k+1 \le q \le N-1$ is the "averaged" position of a subset of the original (tier 0) vertices z_p. In fact, $\mathbf{V}_{N-1}$ is the "averaged" position or "center" of all the vertices in $\mathbf{K}_N$. And $\chi_q = \chi_{q-1} \cup \{j\}$ or $\chi_{q-1} \cup \{2j-1, \; 2j\}$.

(c) the N-th row in the matrix $\mathbf{A}$ is

$$(4.17) \qquad \frac{1}{\sqrt{\sum_{j=1}^{N} \Gamma_j}} \left[\sqrt{\Gamma_1} \quad \sqrt{\Gamma_2} \ldots\ldots\ldots\ldots \sqrt{\Gamma_N} \right].$$

It is now easy to show that the rows of $\mathbf{A}$ form an *orthonormal basis* for $\mathbf{R}^N$ in the following lemmas, thus proving that $\mathbf{A}$ is an *orthogonal* matrix.

LEMMA 4.1. *The first k rows are orthonormal.*

Proof. By inspection, they are orthogonal. A simple calculation for the j-th row, $1 \le j \le k$ gives

$$(4.18) \qquad \mathbf{C}_j^2 \left[\frac{1}{\Gamma_{2j-1}} + \frac{1}{\Gamma_{2j}} \right] = 1 \, .$$

after using (4.14) for $\mathbf{C}_j$.

LEMMA 4.2. *Rows $(k+1)$ to N have euclidean norm 1.*

Proof. It is trivial for row N from the form of (4.17). For the remaining rows, $(k+1)$

to $(N-1)$, simple calculations based on (4.15a, b) show that, respectively

(4.19a)
$$C_q^2 \left[\frac{1}{\Gamma_j} + \frac{\left(\sum_{p \in \chi_{q-1}} \Gamma_p \right)}{\left(\sum_{p \in \chi_{q-1}} \Gamma_p \right)^2} \right]$$
$$= C_q^2 \left[\frac{1}{\Gamma_j} + \frac{1}{\sum_{p \in \chi_{q-1}} \Gamma_p} \right] = 1$$

(4.19b)
$$C_q^2 \left[\frac{\Gamma_{2j-1} + \Gamma_{2j}}{(\Gamma_{2j-1} + \Gamma_{2j})^2} + \frac{1}{\sum_{p \in \chi_{q-1}} \Gamma_p} \right]$$
$$= 1 \, .$$

LEMMA 4.3. *{ Rows 1 to k}⊥ {Rows $k+1$ to N}*

Proof. {Rows 1 to k} ⊥ Row N follows from an easy calculation for the typical j-th row,

(4.20)
$$\frac{\mathbf{C}_j}{\sqrt{\sum_{i=1}^{N} G_i}} \left[-\frac{\sqrt{\Gamma_{2j-1}}}{\sqrt{\Gamma_{2j-1}}} + \frac{\sqrt{\Gamma_{2j}}}{\sqrt{\Gamma_{2j}}} \right] = 0$$

To show that {Rows 1 to k} ⊥ {Rows $k+1$ to $N-1$} we have to consider 3 possibilities for the q-th row (where $k+1 \le q \le N-1$) and the j-th row (where $1 \le j \le k$), namely

1) the $(2j-1)$ and $2j-th$ elements of q-th row are zero,
2) the numbers $(2j-1)$ and $2j$ are in the subset χ_{q-1}
3) these 2 numbers are in the subset $\chi_q \setminus \chi_{q-1}$.

In the first case, Row q ⊥ Row j. In the second case, the inner product (Row j, Row q) reduces to the calculation,

(4.21)
$$\frac{-\mathbf{C}_j \, \mathbf{C}_q}{\sum_{p \in \chi_{q-1}} \Gamma_p} \left[\frac{-\sqrt{\Gamma_{2j-1}}}{\sqrt{\Gamma_{2j-1}}} + \frac{\sqrt{\Gamma_{2j}}}{\sqrt{\Gamma_{2j}}} \right] = 0 \, .$$

In the third case, this inner product takes the form

$$\frac{\mathbf{C}_j\ \mathbf{C}_q}{\Gamma_{2j-1}+\Gamma_{2j}}\left[\frac{-\sqrt{\Gamma_{2j-1}}}{\sqrt{\Gamma_{2j-1}}}+\frac{\sqrt{\Gamma_{2j}}}{\sqrt{\Gamma_{2j}}}\right]=0\ . \tag{4.22}$$

LEMMA 4.4. *{Rows $(k+1)$ to N} are mutually orthogonal.*

Proof. First we show that Row N is orthogonal to the other rows (for both cases in (4.15) by 2 simple calculations of the corresponding inner products,

$$\frac{\mathbf{C}_q}{\sqrt{\sum_{i=1}^{N}\Gamma_i}}\left[\frac{\sqrt{\Gamma_j}}{\sqrt{\Gamma_j}}-\frac{\left(\sum_{p\in\chi_{q-1}}\Gamma_p\right)}{\sum_{p\in\chi_{q-1}}\Gamma_p}\right]=0 \tag{4.23a}$$

$$\frac{\mathbf{C}_q}{\sqrt{\sum_{i=1}^{N}\Gamma_i}}\left[\frac{\Gamma_{2j-1}+\Gamma_{2j}}{\Gamma_{2j-1}+\Gamma_{2j}}-\frac{\left(\sum_{p\in\chi_{q-1}}\Gamma_p\right)}{\sum_{p\in\chi_{q-1}}\Gamma_p}\right]=0 \tag{4.23b}$$

Next, we show that (Row q, Row q') $=0$ where $q'>q$ and $q,q'\in(k+1,\ldots,N-1)$. Because there is only one virtual vertex in each tier ≥ 2 and they are generated consecutively, we deduce that the subsets $\chi_q\subset\chi_{q'}$. This implies that all the non-zero elements in Row q are in column numbers belonging to the set $\chi_{q'-1}$. This is in turn implies that a cancellation must take place in the inner product, whether the q-th row belongs to the first or second cases in (4.15):

$$\frac{\mathbf{C}_q\ \mathbf{C}_{q'}}{\sum_{p\in\chi_{q-1}}G_p}\left[-\frac{\sqrt{\Gamma_j}}{\sqrt{\Gamma_j}}+\frac{\sum_{p\in\chi_{q-1}}(\sqrt{\Gamma_p})(\sqrt{\Gamma_p})}{\sum_{p\in\chi_{q-1}}\Gamma_p}\right]=0 \tag{4.24a}$$

$$\frac{\mathbf{C}_q\ \mathbf{C}_{q'}}{\sum_{p\in\chi_{q-1}}G_p}\left[\frac{-\left(\sqrt{(\Gamma_{2j-1})}\right)^2-(\Gamma_{2j})^2}{\Gamma_{2j-1}+\Gamma_{2j}}+\frac{\sum_{p\in\chi_{q-1}}(\sqrt{\Gamma_p})(\sqrt{\Gamma_p})}{\sum_{p\in\chi_{q-1}}\Gamma_p}\right]=0 \tag{4.24b}$$

Proof of Theorem 4.1. Lemmas 4.1 to 4.4 establish that the matrix $\mathbf{A}$ is *orthogonal* and by observations (iii) and (iv) above, we deduce that $\mathbf{T}_k^s(N)$ is a *symplectic* transformation.

Proof of Corollary 4.1. The corollary follows from the fact that the above proof of Theorem 4.1 did not involve characteristic of the individual members of the equivalence class, $\mathbf{G}_k^s(N)$, but depends on *only* the binary representation of the class.

V. Further Questions and Results. In this section, we take up several questions concerning the further relations between graphs and *symplectic* transformations.

REMARK 5.1. The class of Hamiltonians (1.1) initially considered is too restrictive; the condition of translational invariance can be relaxed. So can the condition that the difference of all possible pairs, $(z_j - z_k)$, must appear in the Hamiltonian. In other words, we can start from a more general graph instead of the complete, $\mathbf{K}_N$. Dropping all of these conditions, we can treat any Hamiltonian which is in the form of a complex function of N complex variables. The next remark reveals that we can even drop the first-order requirement.

REMARK 5.2. The extra symmetry enjoyed by the canonically conjugate variables (real and imaginary parts of $\omega_j = \sqrt{\Gamma_j}\ z_j$) in first-order Hamiltonians is not a necessary part of the procedure and results in this paper. In fact, from the usual formulation for second order problems (where the conjugate of q is a momentum quantity, p), we obtain a significant generalization of the well-known Jacobi coordinates of Celestial Mechanics (cf. H. Pollard [5]). The graphs in this case have vertices in $\mathbb{R}^3$ and the binary operation INTER is now defined in $\mathbb{R}^3$. The procedure for generating the Jacobi coordinates from the spanning tree graphs is slightly different but the method of proofs follows the same approach used above. This problem will be discussed in another paper, [11].

Now, we take up the natural question: With the binary averaging operation fixed (to be INTER), are there other spanning tree graphs besides those given by the equivalence classes, $\mathbf{G}_k^s(N)$ that generates linear *symplectic* transformations of the form, (4.10)?

The answer to this question is *yes* and although these additional graphs are more complicated, they can be obtained from the $\mathbf{G}_k^s(N)$ by a simple procedure. We will not go into details but shall give an illuminating example (cf. figure 3) which was obtained from $\mathbf{G}_2^2(5)$. The proof that these additional tree graphs generate *symplectic* transformations via (4.4) and (4.5) differs only in details from the approach used in Theorem 4.1; it will not be discussed here. Instead, we will give a theorem that elegantly counts the total number of *symplectic* tree graphs, including $\mathbf{G}_k^s(N)$ and the additional ones just described, for given N.

We begin with the definition of a *symplectic* graph:

DEFINITION. A *simple* graph G (with no loops) is said to be *symplectic* if it is the underlying graph of another graph, G', which is generated from K_N by an "averaging" operation, and in turn generates a linear symplectic transformation of the type (4.10). In this paper we have given one class of *symplectic* graphs by fixing the "averaging" operation to be INTER, and the procedure for generating the *symplectic* transformation to be (4.4), (4.5). We remind the readder that a slight abuse of notation in which both the underlying graph, G, and its metrical counterpart, G' (in this case $\mathbf{G}_k^s(N)$) are called *symplectic* graphs, will be used. The reason for choosing the underlying graph, G, in our formal definition is that, the metrical properties of G' produced by INTER are a matter of indifference in the formal theory of graphs. More precisely, these properties are additional structures that lie on the basic concept of a graph, much like the notion of direction of edges [cf. [10]).

In the following theorem, we will count the number of *symplectic* graphs in the class considered here, which is based on INTER and (4.4), (4.5). It is important to note that the count is based *not* on the number of equivalence classes (modulo a permutation) but rather on the actual number of tree graphs, counting each member of an equivalence class. We will use the following properties of these *symplectic* tree graphs in the proof of Theorem 5.1.

LEMMA 5.1. *Every symplectic graph generated by INTER and (4.4), (4.5) satisfies the properties:*

(a) *it is a spanning tree graph (with respect to $\mathbf{K}_N$) with $2N-1$ vertices.*
(b) *it is a binary tree*
(c) *its root is V_{N-1}, the last or highest tiered virtual vertex.*
(d) *its leaves has a one-to-one correspondence with the tier 0 or original vertices in $\mathbf{K}_N$, $\{z_j\}_{j=1}^N$.*

Proof. These properties follow directly from the construction of the *symplectic* graph through the binary operation INTER. This argument works in the case of $\mathbf{G}_k^s(N)$ described in section III, as well as the additional tree graphs generated from the former (cf. discussion earlier in this section and figure 3).

THEOREM 5.1. *The number of symplectic graphs generated by INTER is*

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

Proof. We will adapt a method due to Cayley (cf. Gibbons [5], for counting the numbers of spanning tree graphs in a complete graph, to our purpose. To each *symplectic* 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 in Lemma 5.1; in particular the vertices of degree 1 are in 1-to-1 correspondence with the $\{z_j\}_{j=1}^N$, while the vertices of degree 3 are $\{\mathbf{V}_j\}_{j=1}^{N-2}$, and the only vertex of degree 2 is $\mathbf{V}_{N-1}$. We impose a rank on the vertices of G, in which all the degree 1 vertices, $\{z_j\}_{j=1}^N$ are ranked by the subscript j, all the virtual vertices $\{\mathbf{V}_j\}_{j=1}^{N-1}$ are again ranked by the subscript j, and all the $\{z_j\}$ rank lower than the $\{\mathbf{V}_j\}$.

In choosing the first element in the word for G, we remove the vertex of degree one from G which has the lowest rank, i.e., z_1. The first element is then the subscript of the vertex remaining 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. As we continue 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, is associated with the name-word, $\{1\ 1\ 2\ 2\ 4\ 3\ 3\}$. We 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 subscripts of the virtual vertices. The converse of the above process is also true, that is, we can construct a unique *symplectic* tree G with $(2N-1)$ vertices from a word of length $(2N-3)$ over the alphabet $\{1, \ldots, N-1\}$. (cf. Gibbons [10], page 49, 50).

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

$$(2N-3) \qquad \text{ways to put } (N-1),$$

$$\frac{(2N-4)\,(2N-5)}{2} \qquad \text{ways to put } 1,$$

$$\cdots\cdots\cdots$$

$$\frac{(2)\,(1)}{2} \qquad \text{ways to put } (N-2),$$

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

In conclusion, we raise the following question: Are there other classes of *symplectic* graphs that are constructed from $\mathbf{K}_N$ through some different "averaging" operation? The answers to this question and other related questions concerning the interesting relationship between graph theory and symplectic transformation are not fully known yet and will be explored in forthcoming papers.

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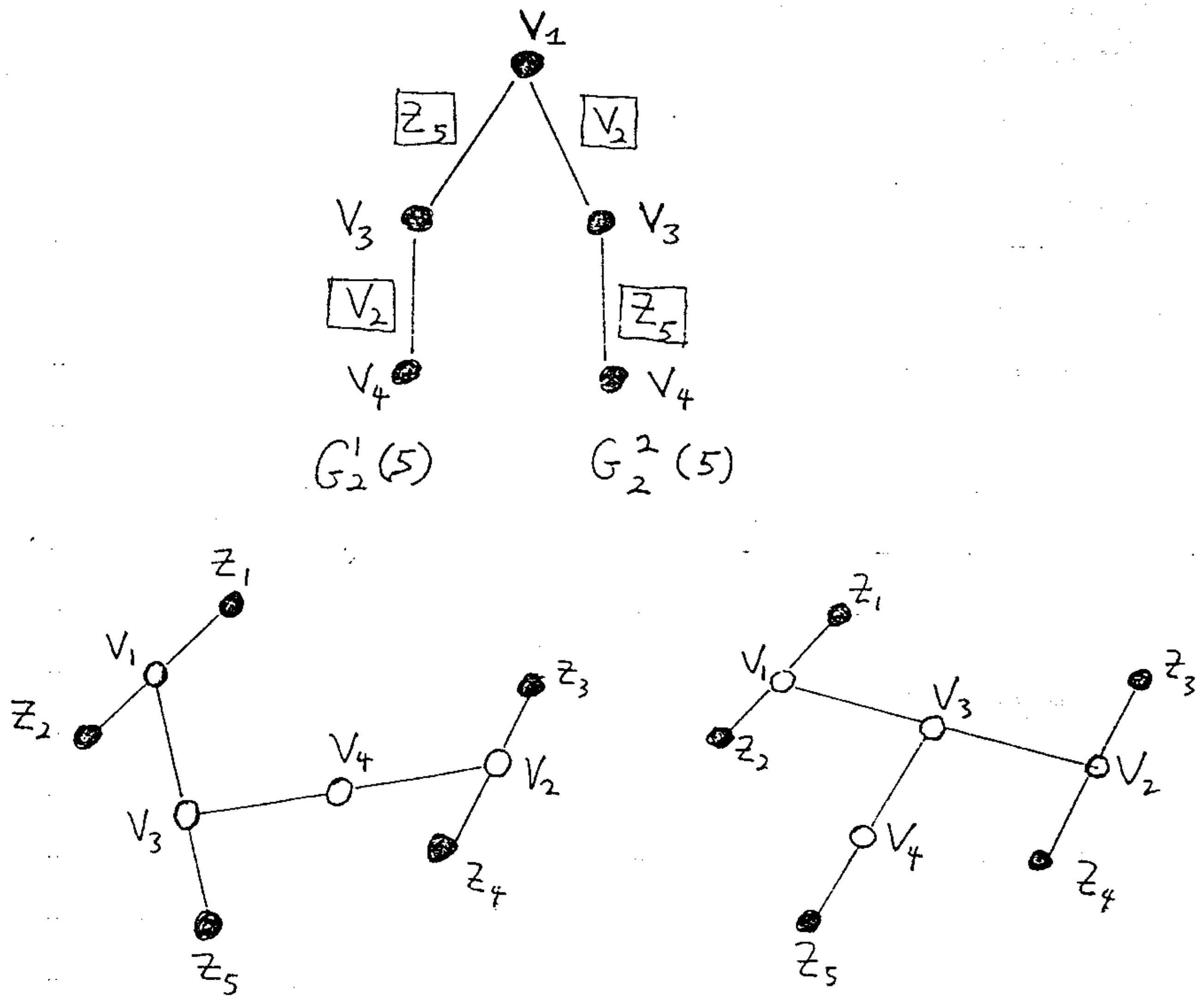

Figure 1: (a) Associated tree, $\mathbf{A}_5^2$
(b), (c) Spanning tree graphs, $\mathbf{G}_2^s(5)$, $s = 1, 2$

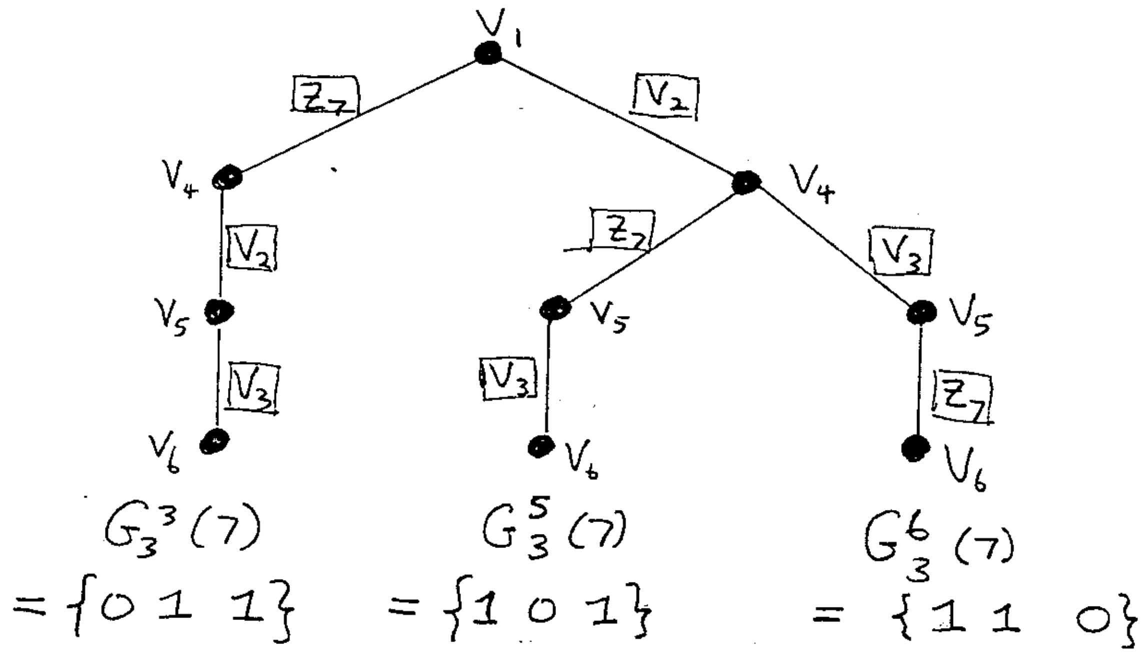

Figure 2: Associated tree, $\mathbf{A}_7^3$ in canonical form.

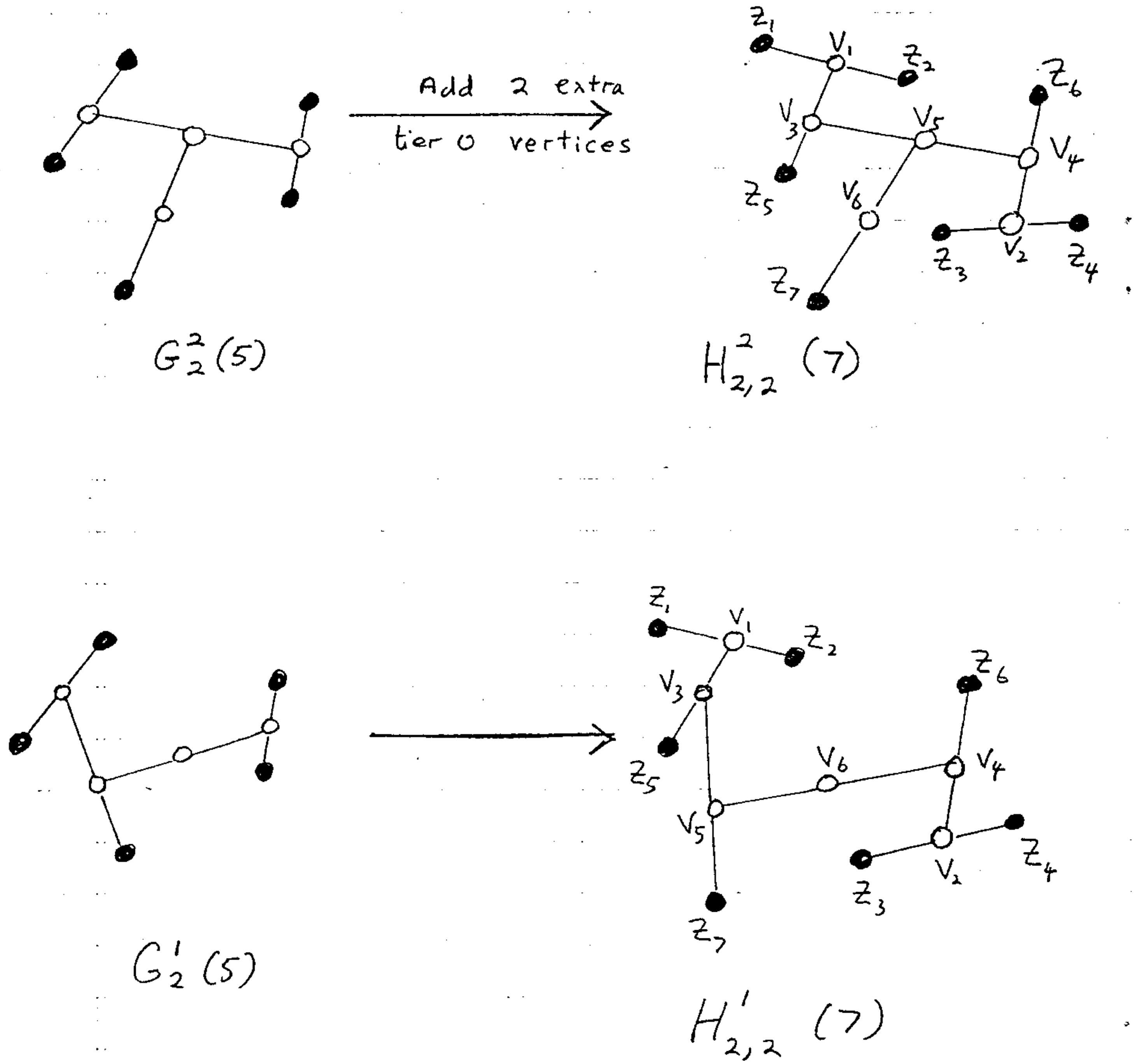

Figure 3: Symplectic Tree Graphs generated by $\mathbf{A}_N^k$ indirectly. From $\mathbf{G}_2^s(5)$, $s = 1, 2$, the corresponding $\mathbf{H}_{2,2}^s(7)$ are generated by adding 2 vertices, keeping $k = 2$ constant but increasing the # of tier 2 virtual vertices to $l = 2$ In both examples, the tier 1 vertices are v_1, v_2 and the tier 2 vertices are v_3, v_4.