CANONICAL TRANSFORMATIONS AND GRAPH THEORY ☆

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In the class of symplectic matrices, two infinite subsets are generated by binary spanning trees. For given N, the procedure begins with the complete graph, K_N to which $N-1$ virtual vertices are added in well-defined ways. Then spanning binary trees that connect the $2N-1$ vertices are obtained and from these trees, explicit formulae give the symplectic matrices. These matrices define linear canonical transformations for N-body problems in vortex dynamics, plasma physics as well as celestial mechanics.

1. Introduction

In the past, there have been many significant applications of graph theory in theoretical physics. Outstanding amongst these are the Feynman diagrams in quantum field theory [1] and Mayer's cluster expansion in statistical mechanics [2]. The results in this note represent a new application of graph theoretical ideas to canonical transformation for classical Hamiltonian systems. More specifically, the transformations discussed here are applicable to a variety of N-body problems in vortex dynamics [3], plasma physics [4] and celestial mechanics [5]. In gravitational N-body problems, isolated cases of these canonical transformations have received the attention of astrophysicists and mathematicians who know them as the Jacobi coordinates [5]. One of the aims here is to give a unified treatment of these transitions in terms of spanning binary trees, that generalizes the Jacobi coordinates. A $2N\times2N$ matrix $\mathbf{M}$ is said to be symplectic if

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

In the context of Hamiltonian mechanics, a transformation in phase space, $T^*(\mathbf{R}^N)$,

$$\boldsymbol{Q}=\boldsymbol{Q}(\boldsymbol{q};\boldsymbol{p}), \quad \boldsymbol{P}=\boldsymbol{P}(\boldsymbol{q};\boldsymbol{p}), \tag{2}$$

is *canonical* if its Jacobian matrix is symplectic. From (2), it is clear that the Jacobian matrix $\mathbf{M}$ has the form

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

where $\mathbf{A}$, $\mathbf{B}$, $\mathbf{C}$, $\mathbf{D}$ are $N\times N$ matrices. Applying (1)–(3) it is clear that the following conditions are equivalent to the above definition of a symplectic matrix:

$$\mathbf{A}^t\mathbf{C},\ \mathbf{B}^t\mathbf{D} \text{ are symmetric } N\times N \text{ matrices}, \tag{4a}$$

$$\mathbf{A}^t\mathbf{D}-\mathbf{C}^t\mathbf{B}=\mathbf{I}_N. \tag{4b}$$

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Also evident is the observation that these conditions for a canonical transformation are independent of the Hamiltonian function.

In this note, we consider two classes of linear canonical transformations; equivalently we discuss a graph-theoretic method for generating symplectic matrices. These matrices fall into two general classes; they take the following forms:

$$\mathbf{M}_1 \begin{bmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{A} \end{bmatrix}, \quad \mathbf{A} \text{ is an } N\times N \text{ real matrix}\,, \tag{5}$$

and

$$\mathbf{M}_2 = \begin{bmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{D} \end{bmatrix}, \quad \mathbf{D} \neq \mathbf{A} \text{ are } 3N\times 3N \text{ real matrices}\,. \tag{6}$$

In the first case, (4a) is satisfied (trivially) while (4b) translates into

$$\mathbf{A}^{\mathrm{t}}\mathbf{A} = \mathbf{I}_N\,. \tag{7}$$

In the other case, (4a) is also trivial and (4b) becomes

$$\mathbf{A}^{\mathrm{t}}\mathbf{D} = \mathbf{I}_{3N}\,. \tag{8}$$

Although these symplectic matrices are identified with canonical transformations independent of the particular Hamiltonian function, to each class of matrices belongs a *natural* family of Hamiltonians. To distinguish them, we will call those associated with $\mathbf{M}_1$ first-order Hamiltonians, and those associated with $\mathbf{M}_2$ second-order Hamiltonians. It turns out that these labels are appropriate in a different sense. The second-order Hamiltonians arise naturally in the N-body problems of celestial mechanics (cf. refs. [5–7]). They involve Newton's second law of motion directly and their Hamilton's equations are obtained from the second-order equations of motion (second-order time derivatives) after the usual reduction [5]. On the other hand, the first-order Hamiltonians, such as those from vortex dynamics [3], and plasma physics [4], do not involve accelerations and forces; their Hamilton's equations are not derived from equations of motion with second-order time derivatives.

We will describe these Hamiltonians explicitly in section 2. In section 3, we show how a *complete graph* K_N can be associated with these Hamiltonians. Next we will describe a procedure for generating spanning tree graphs, starting from K_N. Finally, explicit formulae for the symplectic matrices will be given in terms of the spanning tree graphs. Instead of complete proofs which are published elsewhere [8,9], we give some illuminating examples of our procedure in section 4 of this note. For graph-theoretical concepts (which are essentially self-evident), we refer the reader to refs. [10,11].

2. Hamiltonians

The first-order Hamiltonians described in section 1 have the general form

$$H(\boldsymbol{Z}) = \mathrm{Re}\left\{\sum_{j\neq k=1}^{N} \Gamma_j \Gamma_k F_{jk}(Z_j - Z_k)\right\}, \quad \boldsymbol{Z} = (Z_1, ..., Z_N)\,, \tag{9}$$

where $Z_j \in \mathbb{C}$ give the positions of N particles in the plane, and $\Gamma_j \in \mathbb{R}$ are their "weights". F_{jk} are analytic functions of one complex variable (with the possibility of isolated singularities). The conjugate variables (canonical coordinates) are [#1]

[#1] In this paper, we will focus on "weights" of one sign; the general case is only technically different.

$$q_j=\sqrt{|\Gamma_j|}\,x_j,\quad p_j=\sqrt{|\Gamma_j|}\,y_j,\quad Z_j=x_j+\mathrm{i}y_j\,. \tag{10}$$

A concrete example from vortex dynamics [4] is given by

$$F_{jk}=\text{logarithm} \tag{11}$$

in which the particular branch of the complex logarithm function is immaterial because the Hamiltonian involves only the real part.

The second-order Hamiltonians are the usual N-body Hamiltonians with general potential functions,

$$H(\boldsymbol{q},\boldsymbol{p})=\sum_{j=1}^{N}\frac{|p_j|^2}{2m_j}-U(\boldsymbol{q})\,. \tag{12}$$

where the Euclidean norm in $\mathbb{R}^3$ is

$$|\boldsymbol{p}|^2=(p_j^{(1)})^2+(p_j^{(2)})^2+(p_j^{(3)})^2$$

and the potential has the form

$$U(\boldsymbol{q})=G\sum_{j\neq k}^{N}\frac{m_j m_k}{|q_j-q_k|^l}\,.$$

G is a real constant, m_j are the masses of the particles and

$$|q_j-q_k|^l\equiv[(q_j^{(1)}-q_k^{(1)})^2+(q_j^{(2)}-q_k^{(2)})^2+(q_j^{(3)}-q_k^{(3)})^2]^{1/2}\,,$$

l is a real number greater than zero, and the Newtonian case is obtained when $l=1$.

3. Spanning binary trees and symplectic matrices

Although the symplectic matrices we are concerned with can be discussed without reference to the Hamiltonians in section 2, we want to motivate the introduction of graph-theoretic concepts by starting our discussion with N-body problems with pair-wise (2-body) interactions. Both classes of Hamiltonians in section 2 are of this type.

If we connect all possible pairs of points in the plane given by $\boldsymbol{Z}=(Z_1, ..., Z_N)$ in (9), the resulting picture is the complete graph, K_N. Similarly, for the Hamiltonian (12), we obtain K_N where the vertices are located in $\mathbb{R}^3$. Thus, we are justified in associating a complete graph K_N with the abstract N-body problem with pair-wise interactions. Furthermore, each particle (vertex) has a "weight"; in (9) they are Γ_j (which represents vorticity in vortex dynamics, (11)).

Our procedure consists of three parts: (a) an *averaging* step that defines a binary operation INTER, (b) based on INTER, $N-1$ virtual vertices are added to the original N vertices in K_N to make a spanning tree with $2N-1$ vertices $G_k^j(N)$, and (c) for each virtual vertex in the tree, corresponding rows in the matrices $\mathbf{A}$ and $\mathbf{D}$ (5), (6) are given explicitly by well-defined rules.

The binary operation, INTER is given by

$$\mathrm{V}=\mathrm{INTER}(\mathrm{A},\mathrm{B})=\frac{\Gamma(\mathrm{A})\mathrm{A}+\Gamma(\mathrm{B})\mathrm{B}}{\Gamma(\mathrm{A})+\Gamma(\mathrm{B})},\quad \Gamma(\mathrm{A}),\Gamma(\mathrm{B})\in\mathbb{R};\quad \mathrm{V},\mathrm{A},\mathrm{B}\in\mathbb{C}\,, \tag{13}$$

where $\mathrm{V}=\mathrm{V}_j$ is a new virtual vertex and the arguments A, B can be either a previously generated virtual vertex, e.g. V_h for some $h<j$ or one of the original vertices in K_N, e.g. Z_q, $q=1, ..., N$. To complete step (a), the weight of the new virtual vertex is calculated as follows:

$$\Gamma(\mathrm{V})=\Gamma(\mathrm{A})+\Gamma(\mathrm{B})\,. \tag{14}$$

This operation is governed by the rules

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

(ii) to begin, $k \leqslant [N/2]$ *disjoint* edges in K_N are pre-selected to produce the first k virtual vertices, V_j where $1 \leqslant j \leqslant k$;

(iii) the process stops when there are no eligible pairs of vertices remaining that can be used as arguments of INTER.

The original vertices, Z_q, are said to be in tier 0, while the first k virtual vertices in (ii) are said to be in tier 1 and virtual vertices generated by subsequent applications of INTER are said to be in tiers $\geqslant 2$, according to the number of times INTER has been used.

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

$$V_j = \mathrm{INTER}(Z_{2j-1}, Z_{2j}), \quad j = 1, ..., k . \tag{15}$$

The number of tier-1 vertices is assigned to the index k in the labels $G_k^s(N)$ for the spanning trees with $2N-1$ vertices and A_N^k, the associated tree which will be introduced next.

In order to organize our procedure, we introduce an associated tree A_N^k for each N and each $k \leqslant [N/2]$. The branches of A_N^k code the different routes for constructing $G_k^s(N)$ from K_N. For given N and $k \leqslant [N/2]$, the associated tree, A_N^k, is constructed according to the rules

(i) the root is always labelled V_1,

(ii) the branches code the generation of virtual vertices in tiers $\geqslant 2$; beginning with V_{k+1} and ending with V_{N-1}, the *vertices* of A_N^k below the *root* appear in the same order (increasing subscript) on each branch; it is assumed that the tier-1 vertices V_j for $j = 1, ..., k$ are generated as in (15),

(iii) the *edges* of A_N^k are labelled by boxed vertices consisting of *only* the Z_q, $2k+1 \leqslant q \leqslant N$, and the tier-1 vertices, V_j, $j = 1, ..., k$,

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

We now give an example of the above step for generating spanning trees, which is part (b) of the whole procedure. The example chosen is A_5^2 (cf. fig. 1) where $k = 2$ is the maximum number of tier-1 virtual vertices or equivalently, disjoint edges in the complete graph, K_5. We begin by generating the tier-1 vertices

$$V_1 = \mathrm{INTER}(Z_1, Z_2), \quad V_2 = \mathrm{INTER}(Z_3, Z_4) . \tag{16}$$

The root of A_5^2 is denoted by V_1. From the root there are two distinct ways to generate the tier-2 vertex, V_3. On the right branch (fig. 1),

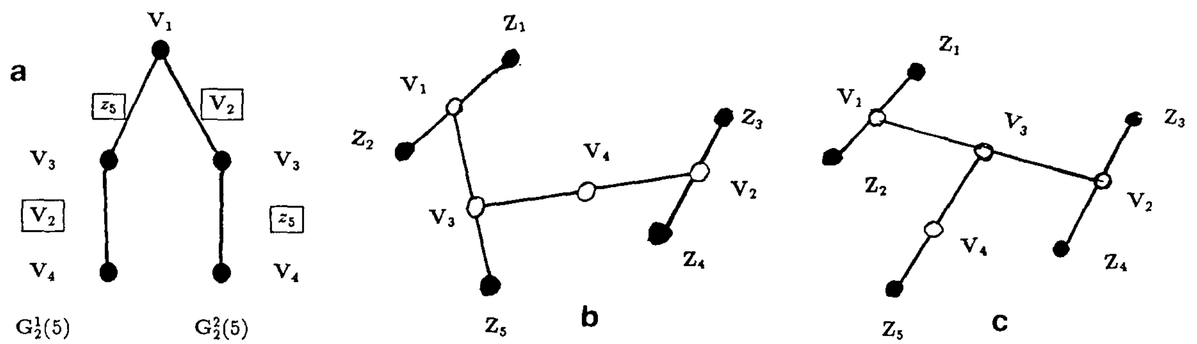

Fig. 1. (a) Associated tree, A_5^2; (b), (c) spanning tree graphs, $G_2^s(5)$, $s = 1, 2$.

$V_3 = \mathrm{INTER}(V_1, V_2)$,

and on the left,

$V_3 = \mathrm{INTER}(V_1, Z_5)$.

This is depicted in the trees, $G_2^s(s)$, where $s=1, 2$ for the left and right branches respectively (cf. figs. 1b, 1c). The next vertex in each branch of A_5^2 is the tier-3 virtual vertex, V_4 on the right,

$V_4 = \mathrm{INTER}(V_3, Z_5)$

and on the left,

$V_4 = \mathrm{INTER}(V_3, V_2)$.

There is now no additional branching in A_5^2 and all 4 virtual vertices in $G_k^s(5)$, $s=1, 2$, have been generated. Clearly, all the tier-0 vertices, Z_q, $q=1, ..., 5$ and the tier-1 vertices, V_j, $j=1, 2$ have been used only once, thereby satisfying the rules that govern INTER.

The two branches of A_5^2 have the following *path representations*,

$$G_2^1(5) = \left\{ \boxed{Z_5}, \boxed{V_2} \right\}, \quad G_2^2(5) = \left\{ \boxed{V_2}, \boxed{Z_5} \right\}, \tag{17}$$

where the boxed quantities denote the edges of A_5^2 to distinguish them from the vertices of $G_2^s(5)$, after which they were named.

The index s in the label $G_k^s(N)$ takes the value of the binary number obtained when the path representation (17) is put in binary form,

$$G_2^1(5) = \{0 \quad 1\}, \quad G_2^2(5) = \{1 \quad 0\}, \tag{18}$$

where 0 denotes a tier-0 vertex, and a 1 denotes a tier-1 vertex. This completes the example A_5^2 and gives a description of parts (a) and (b) of our procedure.

Next, we give the third part (c) of our procedure in which the spanning trees $G_k^s(N)$ are associated with symplectic matrices, $\mathbf{M}_1$ and $\mathbf{M}_2$ (5), (6). We begin with the rules for $\mathbf{M}_1$ and then modify them for $\mathbf{M}_2$.

Let

$$\mathrm{ARG1}(q) = \text{1st argument in INTER that generated } V_q, \text{ the } q\text{th virtual vertex}, \tag{19a}$$

$$\mathrm{ARG2}(q) = \text{2nd argument in the same operation}. \tag{19b}$$

In other words,

$$V_q = \mathrm{INTER}(\mathrm{ARG1}(q), \mathrm{ARG2}(q)), \tag{20}$$

and the "weight" of V_q is

$$\Gamma(V_q) = \Gamma(\mathrm{ARG1}(q)) + \Gamma(\mathrm{ARG2}(q)). \tag{21}$$

We remind the reader that the arguments of INTER are complex numbers that give the position of particles or equivalently, vertices in either $\mathbb{R}^2$ or $\mathbb{R}^3$; the "weights" are real numbers defined by (14).

In the case of $\mathbf{M}_1$, for every virtual vertex V_q in $G_k^s(N)$, we define

$$\rho_q = \left[\frac{\Gamma(\mathrm{ARG1}(q)) \cdot \Gamma(\mathrm{ARG2}(q))}{\Gamma(V_q)} \right]^{1/2} [\mathrm{ARG2}(q) - \mathrm{ARG1}(q)] \tag{22a}$$

for $q=1, ..., N-1$ and

$$\rho_N = \frac{\sum_{j=1}^{N} \Gamma_j Z_j}{\sum_{j=1}^{N} \Gamma_j} . \tag{22b}$$

Since the arguments of INTER are ultimately linear combinations of the tier-0 vertices, Z_j, $j=1, ..., N$, formulae (22) define a real linear transformation on $\mathbb{C}^N$. Recalling that the symplectic coordinates for first-order Hamiltonians (9) are given by the complex number (cf. (10))

$$\omega_j = \sqrt{|\Gamma_j|}\, Z_j, \quad j=1, ..., N , \tag{23}$$

we obtain the desired transformation on $\mathbb{C}^N$ by substituting $\omega_j/\sqrt{|\Gamma_j|}$ for Z_j in (22a,b). The matrix of this transformation is the $N\times N$ real constant matrix $\mathbf{A}$ and $\mathbf{M}_1$ is given by

$$\mathbf{M}_1 = \begin{bmatrix} \mathbf{A} & 0 \\ 0 & \mathbf{A} \end{bmatrix} .$$

$\mathbf{M}_1$, a $2N\times 2N$ real matrix, can be viewed as a transformation from the $2N$ symplectic coordinates, (10), or the real and imaginary parts of (23) to the $2N$ coordinates obtained by taking real and imaginary parts of ρ_q, $q=1, ..., N$.

The main result for $\mathbf{M}_1$ is

Theorem 1. For any N and $k \leqslant [N/2]$, the spanning trees $G_k^s(N)$ generated by INTER via A_N^k define linear canonical transformations (symplectic matrices $\mathbf{M}_1$) which are explicitly given by (22) and (23).

The proof of this theorem is based on verifying that the matrix $\mathbf{A}$ is *orthogonal* for each $G_k^s(N)$. The graph-theoretic details are given in ref. [8].

In the case of $\mathbf{M}_2$, the definitions (19) are valid and the "weights" Γ_j become masses of the particles, m_j. We now modify (22) to take into account the asymmetry between the canonical coordinates and momenta of the second-order Hamiltonians (12). For each virtual vertex, V_j in $G_k^s(N)$, we write

$$Q_j = \mathrm{ARG2}(j) - \mathrm{ARG1}(j) , \tag{24a}$$

$$P_j = \left[\frac{\Gamma(\mathrm{ARG1}(j))\cdot\Gamma(\mathrm{ARG2}(j))}{\Gamma(V_j)}\right] [\dot{\mathrm{ARG}}2(j) - \dot{\mathrm{ARG}}1(j)] , \tag{24b}$$

where ARG1(j), ARG2(j), Q_j, P_j are vectors in $\mathbb{R}^3$, $\Gamma(\;)$ are the masses and $\dot{\mathrm{ARG}}(j)$ denotes the time derivative. This is completed by

$$Q_N = \frac{\sum_{j=1}^{N} m_j q_i}{\sum_{j=1}^{N} m_j}, \qquad P_N = \frac{\sum_{j=1}^{N} p_j}{\sum_{j=1}^{N} m_j} . \tag{24c}$$

The arguments $\dot{\mathrm{ARG}}1(j)$, $\dot{\mathrm{ARG}}2(j)$ are linear combinations of the tier-0 vertices, $q_j \in \mathbb{R}^3$, $j=1, ..., N$ while the time derivatives $\dot{\mathrm{ARG}}1(j)$, $\dot{\mathrm{ARG}}2(j)$ can be written as linear combinations of the conjugate momenta by the substitution

$$\frac{p_j}{m_j} = \dot{q}_j . \tag{25}$$

Therefore, (24) give a linear (real) transformation from $(q_j, p_j) \in \mathbb{R}^{3N}\times\mathbb{R}^{3N}$ to new coordinates $(Q_j, P_j) \in$

$\mathbb{R}^{3N}\times\mathbb{R}^{3N}$. In fact, (24a) defines the $3N\times 3N$ real constant matrix $\mathbf{A}$ and after using (25), the second part (24b) defines the $3N\times 3N$ matrix, $\mathbf{D}$ in $\mathbf{M}_2$ (6).

By (8) the proof [8] of the following theorem is based on checking that $\mathbf{A}^{\mathrm{t}}\mathbf{D}=\mathbf{I}_{3N}$ for every $\mathrm{G}^{\mathrm{s}}_{k}(N)$ generated by the INTER via $\mathbf{A}^{k}_{N}$ from the complete graph K_N (which in this case is located in $\mathbb{R}^3$). As far as graph-theory is concerned, the fact that K_N in this case is in $\mathbb{R}^3$, does not make any difference. The main result for $\mathbf{M}_2$ is

Theorem 2. For any N and $k\leqslant[N/2]$, the spanning trees $\mathrm{G}^{\mathrm{s}}_{k}(N)$ define linear canonical transformations (symplectic matrices $\mathbf{M}_2$) which are explicitly given by (24a,b) and (25).

4. Examples and conclusion

We present two simple examples of canonical transformations generated by our procedure. One of the examples is a symplectic matrix of type one while the other is of type two but they are both generated from the same spanning tree, $G^1_2(5)$ (cf. fig. 1b).

Following the procedure discussed in section 3 (22), for every virtual vertex in $G^1_2(5)$ there belongs a row in the matrix $\mathbf{A}$, given by the complex formulas

$$\rho_1=\left[\frac{\Gamma_1\Gamma_2}{\Gamma_1+\Gamma_2}\right]^{1/2}\left(\frac{\omega_2}{\sqrt{\Gamma_2}}-\frac{\omega_1}{\sqrt{\Gamma_1}}\right),\qquad \rho_2=\left[\frac{\Gamma_3\Gamma_4}{\Gamma_3+\Gamma_4}\right]^{1/2}\left(\frac{\omega_4}{\sqrt{\Gamma_4}}-\frac{\omega_2}{\sqrt{\Gamma_3}}\right),$$

$$\rho_3=\left[\frac{(\Gamma_1+\Gamma_2)(\Gamma_5)}{\Gamma_1+\Gamma_2+\Gamma_5}\right]^{1/2}\left(\frac{\omega_5}{\sqrt{\Gamma_5}}-\frac{\sqrt{\Gamma_1}\,\omega_1+\sqrt{\Gamma_2}\,\omega_2}{\Gamma_1+\Gamma_2}\right),$$

$$\rho_4=\left[\frac{(\Gamma_1+\Gamma_2+\Gamma_5)(\Gamma_3+\Gamma_4)}{\Gamma_1+\Gamma_2+\Gamma_3+\Gamma_4+\Gamma_5}\right]^{1/2}\left(\frac{\sqrt{\Gamma_3}\,\omega_3+\sqrt{\Gamma_4}\,\omega_4}{\Gamma_3+\Gamma_4}-\frac{\sqrt{\Gamma_1}\,\omega_1+\sqrt{\Gamma_2}\,\omega_2+\sqrt{\Gamma_5}\,\omega_5}{\Gamma_1+\Gamma_2+\Gamma_5}\right),$$

$$\rho_5=\frac{\sum_{i=1}^{5}\sqrt{\Gamma_i}\,\omega_i}{\sum_{i=1}^{5}\Gamma_i}\,. \tag{26}$$

$$\mathbf{A}=\begin{bmatrix}
\left[\frac{\Gamma_1\Gamma_2}{\Gamma_1+\Gamma_2}\right]^{1/2} & \left(-\frac{1}{\sqrt{\Gamma_1}}\right. & \frac{1}{\sqrt{\Gamma_2}} & 0 & 0 & \left.0\right)\\
\left[\frac{\Gamma_3\Gamma_4}{\Gamma_3+\Gamma_4}\right]^{1/2} & \left(0\right. & 0 & -\frac{1}{\sqrt{\Gamma_3}} & \frac{1}{\sqrt{\Gamma_4}} & \left.0\right)\\
\left[\frac{(\Gamma_1\Gamma_2)(\Gamma_5)}{\Gamma_1+\Gamma_2+\Gamma_5}\right]^{1/2} & \left(\frac{-\sqrt{\Gamma_1}}{\Gamma_1+\Gamma_2}\right. & -\frac{\sqrt{\Gamma_2}}{\Gamma_1+\Gamma_2} & 0 & 0 & \left.\frac{1}{\sqrt{\Gamma_5}}\right)\\
\left[\frac{(\Gamma_1+\Gamma_2+\Gamma_5)(\Gamma_3+\Gamma_4)}{\Gamma_1+\Gamma_2+\Gamma_3+\Gamma_4+\Gamma_5}\right]^{1/2} & \left(\frac{-\sqrt{\Gamma_1}}{\Gamma_1+\Gamma_2+\Gamma_5}\right. & -\frac{-\sqrt{\Gamma_2}}{\Gamma_1+\Gamma_2+\Gamma_5} & \frac{+\sqrt{\Gamma_3}}{\Gamma_3+\Gamma_4} & \frac{+\sqrt{\Gamma_4}}{\Gamma_3+\Gamma_4} & \left.\frac{-\sqrt{\Gamma_5}}{\Gamma_1+\Gamma_2+\Gamma_5}\right)\\
\left[\frac{1}{\sum_{i=1}^{5}\Gamma_i}\right] & \left(\sqrt{\Gamma_1}\right. & \sqrt{\Gamma_2} & \sqrt{\Gamma_3} & \sqrt{\Gamma_4} & \left.\sqrt{\Gamma_5}\right)
\end{bmatrix} \tag{27}$$

is easily shown to be *orthogonal* by verifying that the rows form an *orthonormal basis* for $\mathbb{R}^5$. Therefore, the matrix $\mathbf{M}_1$ constructed according to (5) is *symplectic* by (7).

The above linear transformation together with infinitely many others generated by the same procedure are guaranteed to be *canonical transformations* by theorem 1. Due to the symmetrical form (5) of these symplectic matrices (where $\mathbf{A}$ appears as diagonal blocks), the most natural Hamiltonians to which these canonical transformations apply are the first-order ones, (9). The symmetry between the "coordinates" q_j and the "moments" p_j is clear since they are essentially the real and imaginary parts of the positions of the particles in the complex plane, (10). In other words, for (9), phase-space can be identified with configuration space. This symmetry sets the first-order problems apart from the second-order Hamiltonians (11), where phase-space $\mathbb{R}^{3N}\times\mathbb{R}^{3N}$ can no longer be identified with configuration space $\mathbb{R}^{3N}$. The second-order problems (11) thus provide the natural setting for applying the canonical transformations associated with symplectic matrices of type two of which an example is given next.

This example of $\mathbf{M}_2$ is generated by applying (24) to each virtual vertex in the graph $G_2^1(5)$. The upper left block $\mathbf{A}$ is given by (24a,c),

$$\mathbf{A}=\begin{bmatrix} -\mathbf{1} & \mathbf{1} & \mathbf{0} & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & -\mathbf{1} & \mathbf{1} & \mathbf{0} \\ -\dfrac{\mathbf{m}_1}{\mathbf{m}_1+\mathbf{m}_2} & -\dfrac{\mathbf{m}_2}{\mathbf{m}_1+\mathbf{m}_2} & \mathbf{0} & \mathbf{0} & \mathbf{1} \\ \dfrac{-\mathbf{m}_1}{\mathbf{m}_1+\mathbf{m}_2+\mathbf{m}_5} & \dfrac{-\mathbf{m}_2}{\mathbf{m}_1+\mathbf{m}_2+\mathbf{m}_5} & +\dfrac{\mathbf{m}_3}{\mathbf{m}_3+\mathbf{m}_4} & \dfrac{+\mathbf{m}_4}{\mathbf{m}_3+\mathbf{m}_4} & \dfrac{-\mathbf{m}_5}{\mathbf{m}_1+\mathbf{m}_2+\mathbf{m}_5} \\ \dfrac{\mathbf{m}_1}{\sum_{j=1}^{5}\mathbf{m}_j} & \dfrac{\mathbf{m}_2}{\sum\mathbf{m}_j} & \dfrac{\mathbf{m}_3}{\sum\mathbf{m}_j} & \dfrac{\mathbf{m}_4}{\sum\mathbf{m}_j} & \dfrac{\mathbf{m}_5}{\sum\mathbf{m}_j} \end{bmatrix}. \tag{28}$$

The lower block $\mathbf{D}$ transforms the old momenta, p_j, into the new momenta, P_j, and is given by (24b,c); each (bold) entry in $\mathbf{A}$ above and $\mathbf{D}$ below represents a 3×3 *diagonal* matrix, for example,

$$-\mathbf{1}\equiv\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix}, \qquad \frac{1}{\mathbf{m}_2}\equiv\begin{bmatrix} m_2^{-1} & 0 & 0 \\ 0 & m_2^{-1} & 0 \\ 0 & 0 & m_2^{-1} \end{bmatrix}.$$

The $3N\times3N$ real constant matrix $\mathbf{D}$ takes the form

$$\begin{bmatrix} \left[\dfrac{m_1m_2}{m_1+m_2}\right] & \left(\dfrac{-1}{\mathbf{m}_1}\right. & \dfrac{1}{\mathbf{m}_2} & \mathbf{0} & \mathbf{0} & \left.\mathbf{0}\right) \\ \left[\dfrac{m_3m_4}{m_3+m_4}\right] & (\mathbf{0} & \mathbf{0} & \dfrac{-1}{\mathbf{m}_3} & \dfrac{1}{\mathbf{m}_4} & \mathbf{0}) \\ \left[\dfrac{(m_1+m_2)m_5}{m_1+m_2+m_5}\right] & \left(\dfrac{-1}{\mathbf{m}_1+\mathbf{m}_2}\right. & \dfrac{-1}{\mathbf{m}_1+\mathbf{m}_2} & \mathbf{0} & \mathbf{0} & \left.\dfrac{1}{\mathbf{m}_5}\right) \\ \left[\dfrac{(m_1+m_2+m_5)(m_3+m_4)}{\sum_{j=1}^{5}m_j}\right] & \left(\dfrac{-1}{\mathbf{m}_1+\mathbf{m}_2+\mathbf{m}_5}\right. & \dfrac{-1}{\mathbf{m}_1+\mathbf{m}_2+\mathbf{m}_5} & \dfrac{1}{\mathbf{m}_3+\mathbf{m}_4} & \dfrac{1}{\mathbf{m}_3+\mathbf{m}_4} & \left.\dfrac{-1}{\mathbf{m}_5+\mathbf{m}_2+\mathbf{m}_5}\right) \\ \left[\dfrac{1}{\sum_{j=1}^{5}m_j}\right] & (\mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1} & \mathbf{1}) \end{bmatrix}. \tag{29}$$

The above symplectic matrix (28), (29) defines a linear canonical transformation for 5-body problems in celestial mechanics where it should be noted that the potentials $U(\boldsymbol{q})$ (12) are not restricted to the gravitational square force-law (cf. ref. [5]). In fact, it gives an example of the so-called Jacobi coordinates, well-known in the 3-body problem [5]. Theorem 2 can be viewed as stating that in the class of $3N\times 3N$ matrices of the form (6) there exists an infinite subset that is generated by binary trees $G_k^{\S}(N)$, and which satisfies the condition for being symplectic, (8). These symplectic matrices, $\mathbf{M}_2$, give a sweeping generalization of the Jacobi coordinates, which are discussed only in special cases (for example the 3-body problem) in the literature.

The canonical transformations defined by $\mathbf{M}_1$ are originally conceived to study clustering phenomena in vortex dynamics [12,13]. Clearly, the range of applications for these transformations is considerably wider; in fact no further restrictions on the form of the functions F_{jk} in (9) are necessary for these transformations to work. Similarly, the Jacobi coordinates defined by $\mathbf{M}_2$ can be applied to the study of clusters in stellar dynamics [14]. In fact, the so-called *cluster coordinates* discussed in McGehee's paper [6] are known to be *symplectic* coordinates [#2]. This provides the point of departure for an extension of the ideas presented to symplectic matrices generated by spanning trees more general than binary ones.

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[#2] Richard McGehee, School of Mathematics, University of Minnesota communicated this to the author.

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