Chin. Ann. of Math.
20B: 1(1999),11-28.

ON THE KINEMATIC GEOMETRY OF MANY BODY SYSTEMS

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Abstract

In mechanics, both classical and quantum, one studies the profound interaction between two types of energy, namely, the kinetic energy and the potential energy. The former can be organized as the kinematic metric on the configuration space while the latter can be represented by a suitable potential function, such as the Newtonian potential in celestial mechanics and the Coulomb potential in quantum mechanics of atomic and molecular physics. In this paper, the author studies the kinematic geometry of n-body systems. The main results are (i) the introduction of a canonical coordinate system which reveals the total amount of kinematic symmetry by an $SO(3) \times O(n-1)$ action in such a canonical coordinate representation; (ii) an in depth analysis of the above kinematic system both in the setting of classical invariant theory and by the technique of equivariant Riemannian geometry; (iii) a remarkably simple formula for the potential function in such a canonical coordinate system which reveals the well-fitting between the kinematic symmetry and the potential energy.

Keywords Kinematic geometry, Many body system, Configuration space
1991 MR Subject Classification 53C, 54E, 81V70
Chinese Library Classification O186.1, O189.11, O413.3

§1. Introduction

The configuration space of a given n-body system consists of the totality of all possible configurations which can be conveniently represented by the n-tuples of position vectors with respect to a suitably chosen origin. Let μ_j be the mass of the j-th particle, $\mu = \sum \mu_j$ be the total mass and $m_j = \mu_j/\mu$ be the percentage of mass of the j-th particle, $\sum m_j = 1$. Following Jacobi, it is natural to introduce the folowing inner product, or rather kinematic metric, on the configuration space

$$\mathbb{R}^{3n} = \{(\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n);\ \mathbf{a}_j \in \mathbb{R}^3\},$$

namely

$$\langle (\mathbf{a}_1, \cdots, \mathbf{a}_n), (\mathbf{b}_1, \cdots, \mathbf{b}_n) \rangle = \sum_{j=1}^{n} m_j \mathbf{a}_j \cdot \mathbf{b}_j, \tag{1.1}$$

so that the kinetic energy can again be written in the same form as that of a single particle, namely

$$T = \sum_{j=1}^{n} \frac{1}{2} \mu_j |\dot{\mathbf{a}}_j|^2 = \frac{1}{2} \mu |(\dot{\mathbf{a}}_1, \cdots, \dot{\mathbf{a}}_n)|^2. \tag{1.2}$$

Manuscript received May 7, 1998.
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By making use of the conservation law of linear momentum, it is always advantageous to fix the origin at the center of mass, thus reducing the configuration space to the $(3n-3)$-dimensional linear subspace defined by the linear condition $\sum m_j \mathbf{a}_j \equiv 0$. We shall denote such a reduced configuration space by M_n. The rotational group, $SO(3)$, fixing the center of mass acts isometrically on M_n and the geometry of $SO(3)$-orbits in M_n is of basic importance in the study of both the classical and the quantum mechanics of such a system. In the special case of 3-body systems the kinematic geometry of mass-triangles has already been thoroughly worked out in [5] and the geometric understanding so obtained plays an important role in the study of both the celestial mechanics and the quantum mechanics of 3-body systems (see [3, 4]).

In this paper, we shall study the kinematic geometry of n-body systems for the general case of $n \geq 4$, namely, the equivariant Riemannian geimetry of $(SO(3), M_n)$. Thus, the basic results of [5] on kinematic geometry of mass-triangles will serve as the prototype of this paper while the main results of this paper are exactly their generalizations to the general case of all $n \geq 4$.

In §2, we introduce a canonical orthogonal decomposition (see (2.3)) which leads to a canonical coordinate system on the configuration space M_n (see Theorem 2.1, §2). Such a canonical coordination establishes a canonical isometry between $(SO(3), M_n)$ and $(SO(3), \mathcal{M}_{3,n-1}(\mathbb{R}))$, thus bringing in an additional kinematic symmetry of $O(n-1)$ corresponding to the right matrix multiplication of $\mathcal{M}_{3,n-1}(\mathbb{R})$ by $O(n-1)$. This is the fundamental starting point which will eventually make a systematic mathematical study n-body problem attainable!

In §3, we take advantage of the algebraic representation of the $O(3) \times O(n-1)$-symmetry on $\mathcal{M}_{3,n-1}(\mathbb{R})$ to provide a rather thorough analysis of its orbital geometry in the setting of classical invariant theory. The results so obtained will then apply to study the orbital geometry of $(SO(3), M_n)$ and its $O(n-1)$-symmetry in §4. The main result of §4 is stated as Theorem 4.1 at the end of §4.

Intuitively speaking, mechanics studies the profound interaction between two types of energy, namely, the kinetic energy and the potential energy. It is the remarkable insight of Laplace and Jacobi that the potential energy can be concisely represnted by a potential function while the kinetic energy can be organized as the kinematic metric on the configuration space, (Jacobi already introduced the concept of Riemannian metric before Riemann!). Hence, it is important to study how well the canonical coordinace system, the additional kinematic symmetry of $O(n-1)$ etc. interact with the potential function. Since most of physically important potential functions such as the Newtonian potential and the Coulomb potential only depend on the pairwise distances among particles, the study of "potential functions" can be reduced to the study of pairwise distance functions $\{r_{ij};\ 1 \leq i < j \leq n\}$. For each given pair of indices (i, j), the zero-set of r_{ij} is a subvariety in M_n consists of those (i, j)-binary collision configurations. Theorem 5.1 proves that r_{ij} is equal to $\sqrt{\frac{m_i+m_j}{m_i m_j}}$ times the distance between the given configuration and the above subvariety of (i, j)-binary collisions, and moreover, the above distance is given by the following simple formula, namely

$$[(\mathbf{u}_{ij} \cdot \mathbf{x}_1^*)^2 + (\mathbf{u}_{ij} \cdot \mathbf{x}_2^*)^2 + (\mathbf{u}_{ij} \cdot \mathbf{x}_3^*)^2]^{1/2},$$

where $\{\mathbf{x}_1^*, \mathbf{x}_2^*, \mathbf{x}_3^*\}$ are the three row vectors of the matrix of canonical coordinates and $\{\mathbf{u}_{ij}\}$ are given by Theorem 6.1 in terms of the mass distribution by explict formulas. The above simple formula of r_{ij} in terms of inner product in $\mathbb{R}^{n-1}$ is truly a wonderful manifestation of the nature's well-fitting between the kinematic geometry and the potential energy. This, of course, will greatly facilitate the study of mechanics of many body systems, both in the classical and in the quantum settings.

§2. A Canonical Orthogonal Decomposition of the Configuration Space; A Canonical Coordinate System and the Emergence of the additional $O(n-1)$ Kinematic Symmetry

Let M_{n-1} be the subspace of M_n with $\mathbf{a}_1 = 0$ while $\mathbb{R}^3_1$ be the subspace of configurations with $\mathbf{a}_2 = \mathbf{a}_3 = \cdots = \mathbf{a}_n$, namely, collisions of the $(n-1)$ particles except the first one.

Lemma 2.1. *M_n is the orthogonal direct sum of M_{n-1} and $\mathbb{R}^3_1$, namely*

$$(\mathbf{a}_1, \cdots, \mathbf{a}_n) = (\mathbf{a}_1, \mathbf{b}_1, \cdots, \mathbf{b}_1) + (0, \mathbf{a}_2 - \mathbf{b}_1, \cdots, \mathbf{a}_n - \mathbf{b}_1), \tag{2.1}$$

where $\mathbf{b}_1 = \frac{-m_1}{1-m_1}\mathbf{a}_1$ and the two configurations of the right-hand side are always orthogonal with respect to the Jacobi inner product (see (1.1)).

Proof. It suffices to check the orthogonality, namely

$$\langle(\mathbf{a}_1, \mathbf{b}_1, \cdots, \mathbf{b}_1), (0, \mathbf{a}_2 - \mathbf{b}_1, \cdots, \mathbf{a}_n - \mathbf{b}_1)\rangle = \sum_{j=2}^{n} m_j(\mathbf{a}_j - \mathbf{b}_1) \cdot \mathbf{b}_1$$

$$= \Big(\sum_{j=2}^{n} m_j \mathbf{a}_j\Big) \cdot \mathbf{b}_1 - (1 - m_1)\mathbf{b}_1 \cdot \mathbf{b}_1 = \Big(\sum_{j=1}^{n} m_j \mathbf{a}_j\Big) \cdot \mathbf{b}_1 = 0. \tag{2.2}$$

Definition 2.1. *Set $\mathbb{R}^3_k$, $1 \le k \le n-1$, to be the subspace of those configurations with $\mathbf{a}_j = 0, j < k$ and $\mathbf{a}_{k+1} = \cdots = \mathbf{a}_n$.*

Corollary 2.1. *All $\mathbb{R}^3_k$, $1 \le k \le n-1$, are $SO(3)$-invariant and one has the following canonical orthogonal decomposition of M_n into the direct sum of $\mathbb{R}^3_k, 1 \le k \le n-1$, namely*

$$M_n = \sum_{k=1}^{n-1} \mathbb{R}^3_k. \tag{2.3}$$

Proof. It follows from Lemma 2.1 by induction on n. Moreover, the components of a given configuration in M_n, $(\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n)$, can be computed inductively as follows:

Set

$$m^{(k)} = \sum_{j=k+1}^{n} m_j, \quad \mathbf{b}^{(k)} = \frac{-1}{m^{(k)}} \sum_{j=1}^{k} m_j \mathbf{a}_j, \quad \mathbf{b}_k = \mathbf{b}^{(k)} - \mathbf{b}^{(k-1)}. \tag{2.4}$$

Then the k-th component of $(\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n)$ in the decomposition of (2.3) is given by

$$(0, \cdots, 0, \mathbf{a}_k - \mathbf{b}^{(k-1)}, \mathbf{b}_k, \cdots, \mathbf{b}_k). \tag{2.5}$$

(Notice that $\mathbf{b}^{(0)} = 0, \mathbf{b}_1 = \frac{-1}{1-m_1} m_1 \mathbf{a}_1$ is the same as that of (2.1) and the sum of the first k components is equal to $(\mathbf{a}_1, \cdots \mathbf{a}_k, b^{(k)}, \cdots, \mathbf{b}^{(k)})$.)

Lemma 2.2. *For $1 \le k \le n-1$, set*

$$\alpha_k = \sqrt{\frac{m_k m^{(k-1)}}{m^{(k)}}}, \quad \mathbf{x}_k = \alpha_k(\mathbf{a}_k - \mathbf{b}^{(k-1)}),$$
$$\iota_k(\mathbf{x}_k) = \alpha_k^{-1}\Big(0, \cdots, 0, \mathbf{x}_k, -\frac{m_k}{m^{(k)}}\mathbf{x}_k, \cdots, -\frac{m_k}{m^{(k)}}\mathbf{x}_k\Big)$$
$$= (0, \cdots, 0, \mathbf{a}_k - \mathbf{b}^{(k-1)}, \mathbf{b}_k, \cdots, \mathbf{b}_k). \tag{2.6}$$

Then

$$\langle \iota_k(\mathbf{x}_k), \iota_k(\mathbf{x}_k)\rangle = |\mathbf{x}_k|^2, \quad \langle \iota_j(\mathbf{x}_j), \iota_k(\mathbf{x}_k)\rangle = 0, \quad j \ne k,$$
$$\sum_{k=1}^{n-1} \iota_k(\mathbf{x}_k) = (\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n). \tag{2.7}$$

Proof. It suffices to verify the first equation of (2.7), the other two equations of (2.7) follow directly from Lemma 2.1, Corollary 2.1 and (2.6)

$$\langle \iota_k(\mathbf{x}_k), \iota_k(\mathbf{x}_k)\rangle = \alpha_k^{-2}|\mathbf{x}_k|^2\Big[m_k + m^{(k)}\Big(\frac{m_k}{m^{(k)}}\Big)^2\Big]$$
$$= |\mathbf{x}_k|^2 \frac{m^{(k)}}{m_k m^{(k-1)}}\Big[m_k + \frac{m_k^2}{m^{(k)}}\Big] = |\mathbf{x}_k|^2. \tag{2.8}$$

(Notice that $m_k + m^{(k)} = m^{(k-1)}$).

A Canonical Coordinate System of M_n

Let $\{\mathbf{x}_k;\ 1 \le k \le n-1\}$ be the set of vectors of Lemma 2.2 canonically associated to a given n-tuple of position vectors in M_n, i.e., $\{\mathbf{a}_j;\ 1 \le j \le n\}$, $\sum m_j \mathbf{a}_j = 0$. Set

$$X = (x_{ik}), \quad 1 \le i \le 3, \quad 1 \le k \le n-1 \tag{2.9}$$

to be the $3 \times (n-1)$ matrix whose k-th column vector is exactly the coordinate vector of $\mathbf{x}_k$ with respect to a fixed chosen Cartesian coordinate system in the physical space. Let $\mathcal{M}_{3,n-1}(\mathbb{R})$ be the space of $3 \times (n-1)$ real matrices equipped with the usual norm, namely

$$|X|^2 = \mathrm{tr} X^t X, \quad X \in \mathcal{M}_{3,n-1}(\mathbb{R}). \tag{2.10}$$

Theorem 2.1. *The above mapping which canonically assign the $3 \times (n-1)$ real matrix $X = (x_{ik})$ to a given configuration in M_n, namely*

$$\{\mathbf{a}_j;\ 1 \le j \le n\} \to \{\mathbf{x}_k;\ 1 \le k \le n-1\} \to X = (x_{ik}) \tag{2.11}$$

is an isometry of M_n onto $\mathcal{M}_{3,n-1}(\mathbb{R})$, in which the $SO(3)$ transformation on M_n corresponds to matrix multiplication by elements of $SO(3)$ from the left.

Proof. By Lemma 2.1 and Lemma 2.2,

$$\langle (\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n), (\mathbf{a}_1, \mathbf{a}_2, \cdots, \mathbf{a}_n)\rangle = \Big\langle \sum_{k=1}^{n-1} \iota_k(\mathbf{x}_k), \sum_{k=1}^{n-1} \iota_k(\mathbf{x}_k)\Big\rangle$$
$$= \sum_{k=1}^{n-1} |\mathbf{x}_k|^2 = \mathrm{tr} X^t X = |X|^2. \tag{2.12}$$

Let g be an element of $SO(3)$ and (g_{ij}) be its matrix with respect to the same fixed chosen coordinate system in the physical space. Then

$$(g\mathbf{a}_1, \cdots g\mathbf{a}_n) = \sum_{k=1}^{n-1} \iota_k(g\mathbf{x}_k) \to (g_{ij}) \cdot (x_{ik}). \tag{2.13}$$

Corollary 2.2. *Let $\{\mathbf{x}_k\}$ (resp. $\{\mathbf{y}_k\}$) be the associated $(n-1)$-tuple of $(\mathbf{a}_j)$ (resp. $(\mathbf{b}_j)$) and X (resp. Y) be the $3\times(n-1)$ matrices with $\{\mathbf{x}_k\}$ (resp. $\{\mathbf{y}_k\}$) as their column vectors. Then*

$$\langle(\mathbf{a}_j),(\mathbf{b}_j)\rangle = \mathrm{tr} Y^t X = \langle X, Y\rangle. \tag{2.14}$$

Proof. By Theorem 2.1

$$\begin{aligned}\langle(\mathbf{a}_j),(\mathbf{b}_j)\rangle &= \frac{1}{2}\{|(\mathbf{a}_j+\mathbf{b}_j)|^2 - |(\mathbf{a}_j)|^2 - |(\mathbf{b}_j)|^2\}\\ &= \frac{1}{2}\{|X+Y|^2 - |X|^2 - |Y|^2\} = \langle X, Y\rangle.\end{aligned} \tag{2.15}$$

Corollary 2.3. *The $SO(3)$-inner product space $(SO(3), M_n)$ has an $SO(3)$-equivariant group of isometries isomorphic to $O(n-1)$ which corresponds to the right-multiplication by orthogonal matrices on $\mathcal{M}_{3,n-1}(\mathbb{R})$.*

Proof. Let g_1 (resp. g_2) be arbitrary elements of $SO(3)$ (resp. $O(n-1)$). It is natural to define the following action of $SO(3)\times O(n-1)$ on $\mathcal{M}_{3,n-1}(\mathbb{R})$ via matrix multiplication, namely

$$(g_1, g_2)X = g_1\cdot X\cdot g_2^t. \tag{2.16}$$

It is easy to check such an action preseve the inner product on $\mathcal{M}_{3,n-1}(\mathbb{R})$, namely

$$\begin{aligned}\langle(g_1,g_2)X,(g_1,g_2)Y\rangle &= \mathrm{tr}(g_1 Y g_2^t)^t(g_1 X g_2^t) = \mathrm{tr}\, g_2 Y^t g_1^t g_1 X g_2^t\\ &= \mathrm{tr}\, g_2 Y^t X g_2^t = \mathrm{tr}\, Y^t X = \langle X, Y\rangle.\end{aligned} \tag{2.17}$$

Therefore, $O(n-1)$ also acts on M_n as an $SO(3)$-equivariant isometric transformation group via the isometric isomorphism of Theorem 2.1.

Remarks. (i) The above additional $O(n-1)$ kinematic symmetry is, of course, an important asset which will greatly facilitate the study of many body problems both in classical and in quantum mechanics.

(ii) The above $SO(3)\times O(n-1)$-action on $\mathcal{M}_{3,n-1}(\mathbb{R})$ can also be considered as the tensor product of $(SO(3),\mathbb{R}^3)$ and $(O(n-1),\mathbb{R}^{n-1})$.

(iii) The isomorphism of Theorem 2.1, i.e., the canonical coordinate system of M_n, deponds on the mass distribution and hence also the ordering of particles in the given n-body system. However, it is not difficult to see that a sole change of ordering of particles will only differ by the right multiplication of a specific element of $O(n-1)$ (see §5 and §6).

(iv) The above canonical coordinate system provides an advantageous coordination of $(SO(3), M_n)$ both for the study of $SO(3)$-equivariant geometry and for the study of $SO(3)$-harmonic analysis on M_n. For one thing, it makes the above studies free from the dependence on the given mass distrubution, wich is, in itself, quite remarkable.

§3. The Orbital Geometry of $(O(3)\times O(n-1), \mathcal{M}_{3,n-1}(\mathbb{R}))$

For the sake of notational simplicity, we shall set $n-1=l$. In this section we shall use the well-known classical invariant theory to analyze the orbital geometry of the $O(3)\times O(l)$-action on $\mathcal{M}_{3,l}(\mathbb{R})$ given by matrix multiplications of $O(3)$ (resp. $O(l)$)) from the left-hand (resp. right-hand) sides, namely

$$(g_1, g_2)X = g_1\cdot X\cdot g_2^t,\quad g_1\in O(3),\quad g_2\in O(l),\quad X\in\mathcal{M}_{3,l}(\mathbb{R}). \tag{3.1}$$

Notice that the above action has an ineffective kernel of $\mathbb{Z}_2 = \{(\pm Id, \pm Id)\}$. Let $\{\mathbf{x}_k;\ 1 \le k \le l\}$ (resp. $\{\mathbf{x}_i^*;\ 1 \le i \le 3\}$) be the column (resp. row) vectors of X. Then the transformation on each individual column vector (resp. row vector) is exactly the usual one.

Let us consider the following commutative diagram of projections to respective orbit spaces, which are geometrical in nature, namely

$$
\begin{array}{ccccc}
 & & \mathcal{M}_{3,l}(\mathbb{R}) & & \\
 & \pi_1 \swarrow & & \searrow \pi_1^* & \\
O(3)\backslash\mathcal{M}_{3,l}(\mathbb{R}) & & & & \mathcal{M}_{3,l}(\mathbb{R})/O(l) \\
 & \pi_2 \searrow & & \swarrow \pi_2^* & \\
 & & O(3)\backslash\mathcal{M}_{3,l}(\mathbb{R})/O(l) & &
\end{array}
\tag{3.2}
$$

On the other hand, by taking advantage of the algebraic definition of the $O(3) \times O(l)$-action, it is natural to introduce the following pair of mappings, namely

$$p_1(X) = X^t X, \quad p_1^*(X) = XX^t, \quad X \in \mathcal{M}_{3,l}(\mathbb{R}), \tag{3.3}$$

which are mappings of $\mathcal{M}_{3,l}(\mathbb{R})$ into real symmetric matrices $S_l(\mathbb{R})$ (resp. $S_3(\mathbb{R})$). Moreover, it is easy to see that

$$p_1(g_1 \cdot X) = p_1(X) \text{ (resp. } p_1^*(X \cdot g_2^t) = p_1^*(X)) \tag{3.4}$$

for all $g_1 \in O(3),\ g_2 \in O(l)$ and $X \in \mathcal{M}_{3,l}(\mathbb{R})$. Therefore, the above two mappings define the following induced mappings

$$
\begin{aligned}
&\rho_1:\ O(3)\backslash\mathcal{M}_{3,l}(\mathbb{R}) \to S_l(\mathbb{R}) \\
&(\text{resp. } \rho_1^*:\ \mathcal{M}_{3,l}(\mathbb{R})/O(l) \to S_3(\mathbb{R}))
\end{aligned}
\tag{3.5}
$$

such that $p_1 = \rho_1 \circ \pi_1$ (resp. $p_1^* = \rho_1^* \circ \pi_1^*$).

Lemma 3.1. (i) *The above two induced mappings ρ_1 and ρ_1^* are both injective.*

(ii) *Assume that $l \ge 3$. Then $\operatorname{Im}\rho_1^*$ consists of those matrices in $S_3(\mathbb{R})$ with non-negative eigenvalues while $\operatorname{Im}\rho_1$ consists of those matrices in $S_l(\mathbb{R})$ with non-negative eigenvalues and at most three of them can be non-zero.*

(iii) *Let $\lambda_1 \ge \lambda_2 \ge \lambda_3 \ge 0$ be the eigenvalues of elements of $\operatorname{Im}\rho_1^*$. Then $(\lambda_i), 1 \le i \le 3$, constitute a coordinate system of $O(3)\backslash\mathcal{M}_{3,l}(\mathbb{R})/O(l)$ and the orbital distance metric on it is given by*

$$d\bar{s}^2 = \frac{1}{4}\sum_{i=1}^{3} \frac{d\lambda_i^2}{\lambda_i}. \tag{3.6}$$

Proof. (i) The injectivity of ρ_1 (resp. ρ_1^*) follows directly from the well-known result of classical invariant theory that the set of inner products, namely

$$\{\mathbf{x}_j \cdot \mathbf{x}_k;\ 1 \le j \le k \le l\} \text{ (resp. } \{\mathbf{x}_h^* \cdot \mathbf{x}_i^*;\ 1 \le h \le i \le 3\}) \tag{3.7}$$

already constitutes a complete set of $O(3)$ (resp. $O(l)$) invariants, and the above sets of inner products are exactly the matrix-coordinates of $X^t \cdot X$ (resp. $X \cdot X^t$). Geometrically, the above fact simply means that they already separate $O(3)$-(resp. $O(l)$-) orbits, namely, the injectivity of ρ_1 (resp. ρ_1^*).

(ii) Notice that

$$\begin{aligned} p_1(Xg_2^t) &= g_2X^t \cdot Xg_2^t = g_2p_1(X)g_2^{-1}, \quad g_2 \in O(l), \\ p_1^*(g_1X) &= g_1X \cdot X^tg_1^t = g_1p_1^*(X)g_1^{-1}, \quad g_1 \in O(3). \end{aligned} \tag{3.8}$$

Therefore, $\mathrm{Im}\,\rho_1$ (resp. $\mathrm{Im}\,\rho_1^*$) are invariant subsets of $S_l(\mathbb{R})$ (resp. $S_3(\mathbb{R})$) with respect to the conjugation transformation of $O(l)$ (resp. $O(3)$), thus consisting of conjugacy classes. On the other hand, real symmetric matrices are always orthogonal conjugate to diagonal matrices and hence each conjugacy class is uniguely characterized by its set of eigenvalues.

Let $\mathbf{s}$ (resp. $\mathbf{t}$) be the $l \times 1$ (resp. 1×3) real matrices with $\{s_j;\ 1 \le j \le l\}$ (resp. $t_j;\ 1 \le i \le 3\}$) as its components. Then

$$\mathbf{s}^tX^t \cdot X\mathbf{s} = \Big|\sum_{j=1}^{l} s_j\mathbf{x}_j\Big|^2 \ge 0, \quad \mathbf{t}X \cdot X^t\mathbf{t}^t = \Big|\sum_{i=1}^{3} t_i\mathbf{x}_i^*\Big|^2 \ge 0. \tag{3.9}$$

Therefore, both X^tX and XX^t are semi-positive definite and hence with all their eigenvalues non-negative. Moreover, X^tX can have at most three non-zero eigenvalues because $\{\mathbf{x}_j;\ 1 \le j \le l\}$ has at most three linearly independent ones among them. On the other hand, it is easy to see that diagonal matrices satisfying the above eigenvalue conditions are clearly elements of $\mathrm{Im}\,\rho_1^*$ (resp. $\mathrm{Im}\,\rho_1$). This completes the proof of (ii).

(iii) Let $\mu_1 > \mu_2 > \mu_3 > 0$ be a generic triple of distinct positive reals and A be the $3 \times l$ matrix with

$$a_{ij} = \mu_i\delta_{ij}, \quad 1 \le i \le 3, \quad 1 \le j \le l \tag{3.10}$$

as its (i, j)-component. Then straightforward computation will show that the isotropy subgroup of A with respect to the $O(3) \times O(l)$-action on $\mathcal{M}_{3,l}(\mathbb{R})$ is given by

$$G_A \simeq O(1)^3 \times O(l-3), \tag{3.11}$$

where

$$O(1)^3 = \left\{ \begin{pmatrix} \pm1 & & O \\ & \pm1 & \\ O & & \pm1 \end{pmatrix} \right\} \subset O(3) \xrightarrow{\delta} O(3) \times O(3) \times O(l-3) \tag{3.12}$$

and δ is the diagonal imbedding of $O(3)$ into $O(3) \times O(3)$. Let F be the fixed point set of the G_A-action on $\mathcal{M}_{3,l}(\mathbb{R})$. Then, it is not difficult to see that

$$F = \{X;\ x_{ij} = r_i\delta_{ij}, \quad r_i \in \mathbb{R}\} \tag{3.13}$$

and moreover, the domain in F defined by $r_1 \ge r_2 \ge r_3 \ge 0$ constitutes a fundamental domain which intersects each $O(3) \times O(l)$-orbit exactly once and perpendicularly. Therefore

$$d\bar{s}^2 = \sum_{i=1}^{3} dr_i^2. \tag{3.14}$$

Notice that $\lambda_i = r_i^2$. Hence

$$dr_i^2 = \frac{1}{4\lambda_i}d\lambda_i^2, \quad d\bar{s}^2 = \frac{1}{4}\sum_{i=1}^{3}\frac{d\lambda_i^2}{\lambda_i}. \tag{3.15}$$

§4. The Orbital Geometry of $(SO(3), M_n)$ and that of its $O(n-1)$-Symmetry

By Theorem 2.1, $(SO(3), M_n)$ is equivariantly isometric to $(SO(3), \mathcal{M}_{3,l}(\mathbb{R}))$, $l = n-1$. Therefore, the $SO(3)$-isometry on M_n can be extended to an $SO(3) \times O(l)$-isometry. Notice that the $O(3) \times O(l)$-action on $\mathcal{M}_{3,l}(\mathbb{R})$ has an ineffective kernel of $\mathbb{Z}_2$ while

$$SO(3) \times O(l) \subset O(3) \times O(l) \to O(3) \times O(l)/\mathbb{Z}_2 \tag{4.1}$$

is an isomorphism onto. Therefore, the above $SO(3) \times O(l)$-isometry on M_n can be isomorphically represented by the $SO(3) \times O(l)$-isometry on $\mathcal{M}_{3,l}(\mathbb{R})$ (see §3).

Let $\overline{M}_n$ be the space of $SO(3)$-orbits in M_n, equipped with the orbital distance metric $d\bar{s}^2$ which measures the shortest distance between orbits. Then, the above $SO(3) \times O(l)$-isometry on M_n induces an $O(l)$-isometry on $(\overline{M}_n, d\bar{s}^2)$ whose orbital distance metric is exactly the one on $O(3)\backslash\mathcal{M}_{3,l}(\mathbb{R})/O(l)$ given by (iii) of Lemma 3.1.

Let $I = \sum\limits_{j=1}^{n} m_j|\mathbf{a}_j|^2$ be the moment of inertia and set $\rho = \sqrt{I}$. Then ρ is exactly the distance between the given configuration and the natural base point of total collision in M_n. Hence, it is the correct measurement of the "size" of the given configuration. By scaling, every configuration other than the total collision can be uniquely normalized to a homothetic configuration of unit size, i.e., with $\rho = 1$. Set M_n^* to be the subspace of $\overline{M}_n$ defined by $\rho = 1$. Then M_n^* equipped with the restricted metric is the geometric representation of all possible shapes (other than that of the total collision) whose kinematic metric provides a natural measurement of the difference in shapes.

Definition 4.1. *The shape space of n-body configurations is defined to be the subspace, M_n^*, of $\overline{M}_n$ with $\rho = 1$ and equipped with the kinematic metric $d\sigma^2 = d\bar{s}^2|M_n^*$.*

It is easy to see that $d\bar{s}^2 = d\rho^2 + \rho^2 d\sigma^2$.

In the known case of $n = 3$, one has the sphericality of shape space (see [5]), namely

$$M_3^* \cong S_+^2\Big(\frac{1}{2}\Big), \quad d\sigma^2 = \frac{1}{4}(d\theta^2 + \sin^2\theta d\phi^2), \tag{4.2}$$

which plays an important role in the study of both the classical and the quantum mechanics of 3-body systems. In this section, we shall determine $(M_n^*, d\sigma^2)$ for the general case of $n \geq 4$. From now on, we shall always assume that $n \geq 4$, set $l = (n-1)$ and identify M_n with $\mathcal{M}_{3,l}(\mathbb{R})$ via the canonical coordinates of §2.

The basic idea of this section is to make use of the $O(l)$-symmetry of $(M_n^*, d\sigma^2)$, namely, to study $(O(l), M_n^*)$ in the setting of equivariant differential geometry. Generally speaking, a given equivariant Riemannian structure (G, N) is uniquely determined by its restriction to the open dense invariant subspace, (G, N_0) consisting of the principal orbits, i.e., orbits of the unique maximal type. Moreover, (G, N_0) is uniquely determined by the following three kinds of orbital geometry, namely

(i) the orbital distance metric which records the normal-part of orbital geometry,

(ii) the tangential part of orbital geometry which records the homogeneous metric on each principal G-orbit,

(iii) the connection on the principal bundle

$$\frac{N(H,G)}{H} \to F(H, N_0) \to N_0/G, \tag{4.3}$$

where H is an arbitrarily chosen and then fixed isotropy subgroup of the principal type; it records the "twisting invariant" of how all the principal G-orbits are fitting together in N_0.

Of course, an important part of the orbital geometry of (G, N_0) is the second fundamental form of each (principal) G-orbits as a submanifold in N_0 and it is conspicuously missing in the above list of basic invariants. The reason for such an omission is that they can be computed in terms of the normal derivatives of (ii). We refer to [1] for a discussion of such basic results on equivariant differential geometry.

Now, let us proceed to determine the above three kinds of orbital geometry (namely, the orbital distance metric, the homogeneous metric of principal orbits and the connection of (4.3)) of the special case of $(O(l), M_n^*)$, $n \geq 4$. First of all, it follows from the fact that F of (3.13) intersects each $O(3) \times O(l)$ orbits prependicularly that the connection of (4.3) becomes trivial in the case of $(O(l), M_n^*)$. This, of course, greatly simplifies the study of the equivariant differential geometry of $(O(l), M_n^*)$.

Set D to be the domian in F of (3.13) defined by the condition $r_1 \geq r_2 \geq r_3 \geq 0$ and $D^*$to be the subset of D with $\sum_{i=1}^{3} r_i^2 = 1$. Let Δ be the image of D^* under the $SO(3)$-orbital projection. Since D is a fundamental domain of $(O(3) \times O(l),\ \mathcal{M}_{3,l}(\mathbb{R}))$ which intersects every $O(3) \times O(l)$-orbits exactly once and prependicularly (see the proof of (iii) of Lemma 3.1), Δ is also a fundamental domain of $(O(l), M_n^*)$ which intersects every $O(l)$-orbits exactly once and prependicularly. Thus

$$D^* \cong \Delta \cong M_n^*/O(l) \text{ (bijection)} \tag{4.4}$$

and they are all isometric to the spherical triangle with the following triple of points as its vertices, namely

$$V_0 = \Big(\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\Big), \quad V_1 = \Big(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0\Big), \quad V_2 = (1, 0, 0). \tag{4.5}$$

Figure 1

Next let us proceed to compute the orbit types of $(O(l), M_n^*)$. Since Δ already constitutes a fundamental domain, it suffices to compute the isotropy subgroups of those points of Δ. We state the result of such a rather straightforward computation as the following Lemma 4.1.

Lemma 4.1. *The isotropy subgroups of points on Δ are given as follows, namely*

(i) $\overline{G}_q = S(O(1)\times O(1)\times O(1))\times O(l-3)$ *if* $q\in\Delta^0$ *(interior of* Δ*),*

(ii) $\overline{G}_q = S(O(1)\times O(2))\times O(l-3)$ *if q belongs to the interior of the spherical arcs* $\overline{V_0V_1}$ *(resp.* $\overline{V_0V_2}$*),*

(iii) $\overline{G}_q = O(1)\times O(1)\times O(l-2)$ *if q belongs to the interior of the spherical arc* $\overline{V_1V_2}$*,*

(iv) $\overline{G}_{V_0} = SO(3)\times O(l-3),\ G_{V_1} = O(2)\times O(l-2),\ G_{V_2} = O(1)\times O(l-1)$.

Proof. Let A be elements of D^* which are the chosen representatives of those $SO(3)$-orbits of Δ, one for each $SO(3)$-orbit. Set $G = O(3)\times O(l)$ and $\overline{G} = O(l)$. Then, straightforward computation will show that

(i) $G_A = O(1)^3\times O(l-3)$ if $r_1 > r_2 > r_3 > 0$,

(ii) $G_A = O(1)\times O(2)\times O(l-3)$ if $r_1 = r_2 > r_3 > 0$ or $r_1 r_2 = r_3 > 0$,

(iii) $G_A = O(1)^2\times O(l-2)$ if $r_1 > r_2 > 0, r_3 = 0$,

(iv) $G_A = O(3)\times O(l-3)$ if $r_1 = r_2 = r_3 = \frac{1}{\sqrt{3}}$,

(v) $G_A = O(2)\times O(l-2)$ if $r_1 = r_2 = \frac{1}{\sqrt{2}},\ r_3 = 0$,

(vi) $G_A = O(1)\times O(l-1)$ if $r_1 = 1, r_2 = r_3 = 0$.

Let q be the $SO(3)$-orbit of A. Then $\overline{G}_q$ and G_A are related as follows, namely

$$\overline{G}_q = SO(3)\cdot(G_A\cap SO(3)\times O(l))/SO(3). \tag{4.6}$$

Therefore, straightforward computation will show that $\overline{G}_q$ are exactly the ones given in Lemma 4.1.

The interior points of Δ represent those principal orbits of $(\overline{G}, M_n^*), \overline{G} = O(l)$, which are homogeneous Riemannian manifolds of the type of

$$O(l)/S(O(1)\times O(1))\times O(l-3). \tag{4.7}$$

Therefore, our next step is to determine the homogeneous Riemannian structres on those principal orbits which can be conveniently parametrized by

$$r_1 > r_2 > r_3 > 0, \quad \sum_{i=1}^{3} r_i^2 = 1. \tag{4.8}$$

Consider $q\in\Delta^0$ as the base point of $\overline{G}(q)\subset M_n^*$. Then the homogeneous Riemannian structure on $\overline{G}(q)$ is uniquely determined by the inner product on its tangent space at the base point $q\in\Delta^0$. The following is a systematic way of computing the above inner product at each $q\in\Delta^0$.

Set $E_{ij},\ i<j$, to be the anti-symmetric $l\times l$ matrix whose only non-zero components are 1 at the (ij)-th place and -1 at the (ji)-th place. Then $\{E_{ij};\ 1\le i\le l\}$ constitutes a basis of the Lie algebra of $O(l)$ while $\{E_{ij};\ 4\le i<j\le l\}$ spans the sub-Lie algebra corresponding to the $O(l-3)$ in $\overline{G}_q$. Therefore

$$\{E_{ij}:\ 1\le i\le 3\ \text{ and } i<j\le l\} \tag{4.9}$$

provides a convenient basis for the quotient space of the Lie algebra of $O(l)$ by the sub-Lie algebra of $O(l-3)$, which can be naturally identified with the tangent space of $\overline{G}(q)$ at the base point $q,\ q \in \Delta^0$. Let $\varphi_{ij}(t) = \operatorname{Exp} tE_{ij}$ be the 1-parameter subgroup in $O(l)$ with E_{ij} as its tangent vector at the identity. It is exactly the 1-parameter subgroup of rotations in the (ij)-plane with unit angular velocity. Restricting the $O(l)$-isometry on M_n^* to each $\varphi_{ij}(t),\ 1 \le i \le 3,\ i < j \le l$, and set K_{ij} to be the Killing vector field generated by such an 1-parameter group of isometries. Then

$$\{K_{ij}(q);\ 1 \le i \le 3,\quad i < j \le l\} \tag{4.10}$$

provides a canonical basis of the tangent space of $\overline{G}(q)$ for each $q \in \Delta^0$. Therefore, it suffices to compute the inner product of the tangent space $\overline{G}(q)$ in terms of the above basis of (4.10). we state the result of such a computation as the following lemma.

Lemma 4.2. *Let $q \in \Delta^0$ and (r_1, r_2, r_3) with the condition of* (4.8) *be its "coordinates". Then*

$$\{K_{ij}(q);\ 1 \le i \le 3,\quad i < j \le l\} \tag{4.11}$$

constitutes an orthogonal basis of the tangent space of $\overline{G}(q)$ at the base point q while their lengths are given as follows

$$\begin{aligned}&\text{(i) } |K_{ij}(q)| = r_i, \quad if\ 1 \le i \le 3, \quad j \ge 4,\\ &\text{(ii) } |K_{ij}(q)| = \frac{r_i^2 - r_j^2}{\sqrt{r_i^2 + r_j^2}}, \quad if\ 1 \le i < j \le 3.\end{aligned} \tag{4.12}$$

Proof. Let π be the orbital projection of $(SO(3), \mathcal{M}_{3,l}(\mathbb{R}))$ and A be the $3 \times l$ matrix with $a_{ij} = r_i\delta_{ij}$. Then $q = \pi(A)$ and it is convenient to lift the computation up to the level of $\mathcal{M}_{3,l}(\mathbb{R})$, namely, one has

$$K_{ij}(q) = d\pi(A \cdot E_{ij}^t), \tag{4.13}$$

Moreover, $K_{ij}(q)$ can be identified with the normal component of $A \cdot E_{ij}^t$ to the $SO(3)$-orbit of A such that the inner products among $\{K_{ij}(q)\}$ are the same as that among their normal components.

The tangent sapce of $SO(3)(A)$ is spanned by the following three $3 \times l$-matrices, namely

$$\begin{pmatrix} 0 & r_2 & 0 & \\ -r_1 & 0 & 0 & O \\ 0 & 0 & 0 & \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & r_3 & \\ 0 & 0 & 0 & O \\ -r_1 & 0 & 0 & \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 & \\ 0 & 0 & r_3 & O \\ 0 & -r_1 & 0 & \end{pmatrix}. \tag{4.14}$$

Therefore, it is straightforward to check that the normal components of $AE_{ij}^t,\ 1 \le i \le 3,\ i < j \le l$ are, in fact, orthogonal to each other. Moreover, simple computation will show that the lengths of their normal components are given by (4.12).

Summarizing the results of this section, we state the main result on the geometry of $(M_n^*, d\sigma^2)$ as the following theorem, namely

Theorem 4.1. *The shape of n-body systems M_n^* equipped with the kinematic metric $d\sigma^2$ has an isometry group isomorphic to $O(n-1)$, having the following basic equivariant geometric structures which uniquely determined the Riemannian manifold $(M_n^*, d\sigma^2)$, namely*

(i) *The orbit space $M_n^*/O(n-1)$ equipped with the orbital distance metric is isometric to the spherical triangle with $\frac{\pi}{2}, \frac{\pi}{3}$ and $\frac{\pi}{4}$ as its three inner angles.*

(ii) *The interior points of the above spherical triangle represent principle $O(l)$-orbits which are homogeneous spaces of the type of $O(n-1)/S(O(1) \times O(1) \times O(1)) \times O(n-4)$ (see Lemma* 4.1.).

(iii) *The homogeneous Riemannian metrics on all principal orbits are given by Lemma 4.2, solely in terms of the natural parameters* $r_1 > r_2 > r_3 > 0$ *with* $\sum r_i^2 = 1$ (*see* (4.13)).

Remarks. (i) In the general case of $n \geq 5$, the isotropy representation of $S(O(1)\times O(1)\times O(1))\times O(n-4)$ of the above type of homogeneous space splits into six non-equivalent irreducible ones, three of them 1-dimensional and three of them $(n-4)$-dimensional. Therefore, a homogeneous Riemannian metric on such type of homogeneous differentiable manifold is uniquely determined by six positive number measuring the sizes in each of the six irreducible tangent subspaces.

(ii) Δ^0 intersets every principal orbit of $(O(n-1), M_n^*)$ at exatly one point and perpendicularly. Moreover, the open submanifold consisting of the totality of principal orbits is differentiably the product of Δ^0 and the homogeneous space $O(n-1)/H$, while the Riemannian structure is described by the six size function given in Lemma 4.2.

(iii) At the boundary points of Δ, some of the six size functions become zero and the principal orbit shrinks to lower dimensional ones.

§5. The Configuration Associated to the Family of Binary Collision Subvarieties and the Fundamental Formula of Potential Functions

In the study of mechanics of many body systems, the congiguration space equipped with the kinematic metric provides the geometric representation of the kinetic emergy while the driving force of the mechanical system is usually represented by the potential function such as the Newtonian potential function in the case of celestial mechanics and Coulomb potential function in the case of quantum mechanics of atomic or molecular physics. In this section, we shall investigate the potential functions of n-body systems in the setting of canonical coordinate system and the kinematic geometry. We shall only consider those potential functions which only depend on the pairwise distances among the n particles in a certain specific way such as the Newtonian and the Coulomb potentials. Therefore, it is important to study the pairwise distances $\{r_{ij};\ 1 \leq i < j \leq n\}$ as functions of the canonical coordinates of §2.

In the special case of $(i,j) = (n-1,n), \mathbf{x}_{n-1}$ is, by definition, a vector along the interval joining the $(n-1)$-th and the n-th partiales. Moreover, one has (see (2.6) and (2.7))

$$\begin{aligned}|\mathbf{x}_{n-1}|^2 &= m_{n-1}\Big(\frac{m_n}{m_{n-1}+m_n} r_{n-1,n}\Big)^2 + m_n\Big(\frac{m_{n-1}}{m_{n-1}+m_n} r_{n-1,n}\Big)^2 \\ &= \frac{m_{n-1}m_n}{m_{n-1}+m_n} r_{n-1,n}^2. \end{aligned} \tag{5.1}$$

Therefore, for the special case of $(i,j) = (n-1,n)$, the formula that expresses $r_{n-1,n}$ as a function of the canonical coordinates is simply the following

$$r_{n-1,n} = \sqrt{\frac{m_{n-1}+m_n}{m_{n-1}m_n}}(x_{1,n-1}^2 + x_{2,n-1}^2 + x_{3,n-1}^2)^{1/2}, \tag{5.2}$$

Due to the fact that the construction of $\{\mathbf{x}_k;\ 1 \leq k \leq n-1\}$ from a given configuration $\{\mathbf{a}_j;\ 1 \leq j \leq n\}$ does depend on the ordering of positive vectors in a rather essential way, the above simple formula for the special case of $(n-1,n)$ can not readily be generalized in a simple manner. Observe that the geometry of $(SO(3), M_n)$ is certainly independent of the choice of ordering of the particles. It is natural to seek the generalization of formula (5.2) (i.e., from the special case of $r_{n-1,n}$ to the general case of $r_{i,j}$) via the following "geometry meaning" of $|\mathbf{x}_{n-1}|$:

The subset in M_n defined by the condition $\mathbf{x}_{n-1} = 0$ is exactly subvariety consisting of those configurations with $\mathbf{a}_{n-1} = \mathbf{a}_n$, i.e., the subvariety of binary collision of type $(n-1, n)$, while the geometric meaning of $|\mathbf{x}_{n-1}|$ is exactly the shortest distance between the given configuration with $X = (x_{ik})$ as its canonical coordinate and the above subvariety $B_{n-1,n}$. Therefore the general formula for $r_{i,j}$ must be of the same geometric form as that of $r_{n-1,n}$, namely

$$r_{i,j} = \sqrt{\frac{m_i + m_j}{m_i m_j}} \text{ (the distance between } X \text{ and } B_{i,j}), \tag{5.2'}$$

where $B_{i,j}$ is the subvariety consisting of those binary collisions of type (i,j), i.e., with $\mathbf{a}_i = \mathbf{a}_j$. Of course, the problem remains to be what is the formula of the distance between X and $B_{i.j}$?

Let us first establish the following basic feature of such subvarieties of binary collisions.

Lemma 5.1. *For each given pair of indices $1 \le i < j \le n$, there exists a unit vector*

$$\mathbf{u}_{ij} = (c_{ij}^{(1)}, c_{ij}^{(2)}, \cdots, c_{ij}^{(n-1)}) \in \mathbb{R}^{n-1}, \tag{5.3}$$

which is uniquely determined by the given mass-distribution up to a sign, such taht the subvariety, B_{ij} of (i,j)-binary collision is given by the condition

$$\sum_{k=1}^{n-1} c_{ij}^{(k)} \mathbf{x}_k = 0. \tag{5.4}$$

Proof. Recall that (see Lemma 2.2)

$$\mathbf{x}_k = \sqrt{\frac{m_k m^{(k-1)}}{m^{(k)}}} \Big(\mathbf{a}_k + \frac{1}{m^{(k-1)}} \sum_{j=1}^{k-1} m_j \mathbf{a}_j\Big), \quad m^{(k-1)} = \sum_{j=k}^{n} m_j, \tag{5.5}$$

The above set of linear relationships can be regarded as the equations of coordinate transfomation between two sets of $(n-1)$ independent 3-dimensional vector-variables, namely

$$\begin{aligned} &\{\mathbf{a}_j;\ 1 \le j \le n-1\} \leftrightarrow \{\mathbf{x}_k;\ 1 \le k \le n-1\} \\ &(\text{resp.}\{\mathbf{a}_j;\ 1 \le j \le n-2, \text{ and } \mathbf{a}_n\} \leftrightarrow \{\mathbf{x}_k;\ 1 \le k \le n-1\}). \end{aligned} \tag{5.6}$$

Moreover, the system of linear equations (5.5) has a lower triangular matrix of coefficients and hence, straightforward step-wise substitutions will provide the linear expressions of the $\{\mathbf{a}_j\}$ in terms of $\{\mathbf{x}_k\}$. Therefore, the linear equation $\mathbf{a}_i = \mathbf{a}_j$ corresponds to a linear equation among the vector-variables $\{\mathbf{x}_k\}$. Of course, one may normalize the coefficients of such a linear equation of $\{\mathbf{x}_k\}$ so that their squares add up to 1, namely

$$\sum_{k=1}^{n-1} c_{ij}^{(k)} \mathbf{x}_k = 0, \quad \sum_{k=1}^{n-1} (c_{ij}^{(k)})^2 = 1. \tag{5.7}$$

This proves the existence of $\mathbf{u}_{ij}$ of (5.3) such that the subvariety of (i,j)-binary collisions, $B_{i,j}$ is given by the condition of (5.4).

Remark. Let $\mathbb{R}_{ij}^{n-2}$ be the prependicular hyperplane of $\mathbf{u}_{ij}$ and represent $\mathcal{M}_{3,n-1}(\mathbb{R})$ as $\mathbb{R}^3 \otimes \mathbb{R}^{n-1}$ in the usual way. Then $B_{ij} = \mathbb{R}^3 \otimes \mathbb{R}_{ij}^{n-2}$.

Definition 5.1. *The collection of* $\frac{1}{2}n(n-1)$ *hyperplances* $\{\mathbb{R}_{ij}^{n-2};\ 1 \le i < j \le n\}$ *in* $\mathbb{R}^{n-1}$ *is called the associated configuration to the family of binary collision subvarieties in* M_n.

Theorem 5.1. *Let* $r_{ij}, 1 \le i < j \le n$, *be the distance between the* i*-th and the* j*-th particle and* $\{\mathbf{x}_1^*, \mathbf{x}_2^*, \mathbf{x}_3^*\}$ *be the row vectors of the matrix of canonical coordinates. Then*

$$r_{ij} = \sqrt{\frac{m_i + m_j}{m_i m_j}}[(\mathbf{u}_{ij} \cdot \mathbf{x}_1^*)^2 + (\mathbf{u}_{ij} \cdot \mathbf{x}_2^*)^2 + (\mathbf{u}_{ij} \cdot \mathbf{x}_3^*)^2]^{1/2}, \tag{5.8}$$

Proof. It follows from Lemma 5.1 that the distance between the configuration with $X = (x_{ik})$ as its matrix of canonical coordintes and the subvariety of (i, j)-binary collisions is exactly given by

$$[(\mathbf{u}_{ij} \cdot \mathbf{x}_1^*)^2 + (\mathbf{u}_{ij} \cdot \mathbf{x}_2^*)^2 + (\mathbf{u}_{ij} \cdot \mathbf{x}_3^*)^2]^{1/2}. \tag{5.9}$$

Hence, by (5.2'), r_{ij} is given by (5.8).

Remark. The pairwise distances r_{ij} are clearly invariant under the action of $SO(3)$. Notice that the induced transformation of $SO(3)$ on the 3×3 symmetric matrix $XX^t = (\mathbf{x}_i^* \cdot \mathbf{x}_j^*)$ is exactly the conjugation. Therefore, under the $SO(3)$-action, every X can be transformed to such a matrix whose row vectors are orthogonal to each other and $|\mathbf{x}_1^*|^2 \ge |\mathbf{x}_2^*|^2 \ge |\mathbf{x}_3^*|^2$. Hence it is advantageous to restrict to te above subset of M_n for the purpose of computing the potential functions. In fact, this is a simple way of making use of the $SO(3)$-invariance of the distance functions $\{r_{ij}\}$, thus already effectively reducing the computation down to the level of $\overline{M}_n$.

§6. The Explicit Formula of $\mathbf{u}_{ij}$ in Terms of the Given Mass Distribution

In this section, we shall proceed to compute the explicit formula of $\mathbf{u}_{ij}$, namely, its $(n-1)$ components $c_{ij}^{(k)},\ 1 \le k \le (n-1)$, in terms of the given mass distribution $\{m_j, 1 \le j \le n\}$. By Lemma 5.1, such $\frac{1}{2}n(n-1)$ unit vectors $\{\mathbf{u}_{ij};\ 1 \le i < j \le n\}$ are unique up to a sign. Let us begin with recalling the defining relations between the n-tuple of position vectors $\{\mathbf{a}_j;\ 1 \le j \le n\}$ and the $(n-1)$-tuple of column vectors $\{\mathbf{x}_k;\ 1 \le k \le (n-1)\}$ of its matrix of canonical coordinates. Set

$$m^{(k)} = \sum_{j=k+1}^{n} m_j, \quad \alpha_k = \sqrt{\frac{m_k m^{(k-1)}}{m^{(k)}}}. \tag{6.1}$$

Then

$$\mathbf{x}_k = \alpha_k\Big(\mathbf{a}_k + \frac{1}{m^{(k-1)}}\sum_{j=1}^{k-1} m_j \mathbf{a}_j\Big), \quad 1 \le k \le n-1. \tag{6.2}$$

The above set of $(n-1)$ linear equations together with the additional one of $\sum\limits_{j=1}^{n} m_j \mathbf{a}_j = 0$ enable us to solve the n-tuple of vectors $\{\mathbf{a}_j;\ 1 \le j \le n\}$ in terms of linear expressions of $\{\mathbf{x}_k;\ 1 \le k \le n-1\}$.

Lemma 6.1. *For* $1 \le k \le n-1$,

$$\mathbf{a}_k = \alpha_k^{-1}\mathbf{x}_k - \sum_{j=1}^{k-1} \frac{m_j}{m^{(j)}} \alpha_j^{-1} \mathbf{x}_j \tag{6.3}$$

and

$$\mathbf{a}_n = -\frac{m_{n-1}}{m_n}\alpha_{n-1}^{-1}\mathbf{x}_{n-1} - \sum_{j=1}^{n-2}\frac{m_j}{m^{(j)}}\alpha_j^{-1}\mathbf{x}_j \tag{6.3'}$$

Proof. In the begining case of $k = 1$,

$$\mathbf{x}_1 = \alpha_1\mathbf{a}_1 \Longrightarrow \mathbf{a}_1 = \alpha_1^{-1}\mathbf{x}_1. \tag{6.4}$$

Next let us discuss the cases of $1 < k \leq n-1$. By (6.2),

$$\mathbf{a}_k = \alpha_k^{-1}\mathbf{x}_k - \frac{1}{m^{(k-1)}}\sum_{j=1}^{k-1} m_j\mathbf{a}_j. \tag{6.5}$$

Therefore, it suffices to show that

$$\frac{1}{m^{(k-1)}}\sum_{j=1}^{k-1} m_j\mathbf{a}_j = \sum_{j=1}^{k-1}\frac{m_j}{m^{(j)}}\alpha_j^{-1}\mathbf{x}_j, \quad 1 \leq k \leq n-1. \tag{6.6}$$

Again, the starting case of $k = 2$ is quite obvious, namely

$$\frac{1}{m^{(1)}}m_1\mathbf{a}_1 = \frac{m_1}{m^{(1)}}\alpha_1^{-1}\mathbf{x}_1 \text{ (by (6.4))}. \tag{6.6_2}$$

Now, let us proceed to prove (6.6) by induction on k, namely, to show that $(6.6)_k \Longrightarrow (6.6)_{k+1}$ provided $k + 1 \leq n - 1$,

$$\begin{aligned}\frac{1}{m^{(k)}}\sum_{j=1}^{k} m_j\mathbf{a}_j &= \frac{m_k}{m^{(k)}}\Big(\alpha_k^{-1}\mathbf{x}_k - \frac{1}{m^{(k-1)}}\sum_{j=1}^{k-1} m_j\mathbf{a}_j\Big) + \frac{1}{m^{(k)}}\sum_{j=1}^{k-1} m_j\mathbf{a}_j \\ &= \frac{m_k}{m^{(k)}}\alpha_k^{-1}\mathbf{x}_k + \frac{1}{m^{(k)}}\Big[1 - \frac{m_k}{m^{(k-1)}}\Big]\sum_{j=1}^{k-1} m_j\mathbf{a}_j \\ &= \frac{m_k}{m^{(k)}}\alpha_k^{-1}\mathbf{x}_k + \frac{1}{m^{(k-1)}}\sum_{j=1}^{k-1} m_j\mathbf{a}_j \\ &= \frac{m_k}{m^{(k)}}\alpha_k^{-1}\mathbf{x}_k + \sum_{j=1}^{k-1}\frac{m_j}{m^{(j)}}\alpha_j^{-1}\mathbf{x}_j = \sum_{j=1}^{k}\frac{m_j}{m^{(j)}}\alpha_j^{-1}\mathbf{x}_j. \end{aligned} \tag{6.7}$$

Finally, let us prove the special case of (6.3'). Using the condition of $\sum\limits_{j=1}^{n} m_j\mathbf{a}_j = 0$, one has

$$m_{n-1}\Big(\mathbf{a}_{n-1} + \frac{1}{m^{(n-2)}}\sum_{j=1}^{n-2} m_j\mathbf{a}_j\Big) + m_n\Big(\mathbf{a}_n + \frac{1}{m^{(n-2)}}\sum_{j=1}^{n-2} m_j\mathbf{a}_j\Big) = 0. \tag{6.8}$$

Therefore

$$\begin{aligned}\mathbf{a}_n &= -\frac{m_{n-1}}{m_n}\Big(\mathbf{a}_{n-1} + \frac{1}{m^{(n-2)}}\sum_{j=1}^{n-2} m_j\mathbf{a}_j\Big) - \frac{1}{m^{(n-2)}}\sum_{j=1}^{n-2} m_j\mathbf{a}_j \\ &= -\frac{m_{n-1}}{m_n}\alpha_{n-1}^{-1}\mathbf{x}_{n-1} - \sum_{j=1}^{k-2}\frac{m_j}{m^{(j)}}\alpha_j^{-1}\mathbf{x}_j. \end{aligned} \tag{6.9}$$

Remark. Notice that

$$\frac{m_j}{m^{(j)}}\alpha_j^{-1} = \sqrt{\frac{m_j}{m^{(j)}m^{(j-1)}}}, \quad -\frac{m_{n-1}}{m_n}\alpha_{n-1}^{-1} = -\sqrt{\frac{m_{n-1}}{m_n(m_{n-1}+m_n)}}. \tag{6.10}$$

With Lemma 6.1 at hand, it is a simple matter to write down the defining equations of $B_{ij},\ 1 \le i < j \le n$, namely, the linear equation of $\{\mathbf{x}_k;\ 1 \le k \le n-1\}$ corresponding to the linear condition $\mathbf{a}_i - \mathbf{a}_j = 0$. We state the result as the following theorem, namely

Theorem 6.1. *Set*

$$\beta_k = \sqrt{\frac{m_k}{m^{(k)} m^{(k-1)}}}, \quad \alpha_k = \sqrt{\frac{m_k m^{(k-1)}}{m^{(k)}}}, \quad m^{(k)} = \sum_{j=k+1}^{n} m_j.$$

Then the (i,j)-binary collision subvariety, B_{ij}, consists of those configurations whose column vectors of the matrix of canonical coordinates $\{\mathbf{x}_k;\ 1 \le k \le n-1\}$ satisfy the following linear equation, namely

$$(\alpha_i^{-1} + \beta_i)\mathbf{x}_i + \sum_{h=i+1}^{j-1} \beta_h \mathbf{x}_h - \alpha_j^{-1}\mathbf{x}_j = 0, \quad 1 \le i < j < n \tag{6.11}$$

(*resp.*

$$(\alpha_i^{-1} + \beta_i)\mathbf{x}_i + \sum_{h=k+1}^{n-2} \beta_h \mathbf{x}_h + \sqrt{\frac{m_{n-1}}{m_n(m_{n-1}+m_n)}}\mathbf{x}_{n-1} = 0, \tag{6.11'}$$

for the special cases of $j = n$). Correspondingly, the unit vector $\mathbf{u}_{ij}$ of Lemma 5.1 is given by

$$\mathbf{u}_{ij} = \mathbf{w}_{ij}/|\mathbf{w}_{ij}|, \tag{6.12}$$

where $\mathbf{w}_{ij}$ is the coefficient vector of (6.11) (*resp.* (6.11')) *in case $j = n$).*

Proof. The (i,j)-binary collision subvariety B_{ij} is, by definition, given by the condition $\mathbf{a}_i - \mathbf{a}_j = 0$. Therefore Theorem 6.1 follows directly from Lemma 6.1.

§7. Concluding Remarks

The kinematic geometry of n-body systems that we discussed in this paper is, of course, just the starting point of our long journey of a systematic study of the mechanics of n-body system, both in celestial mechanics and in quantum mechanics. However, it already constitutes a solid well-fitting geometric foundation which makes a systematic study of n-body problems in both celestial mechanics and in atomic and molecular quantum theory, at all, feasible. The canonical coordinate system, the additional kinematic symmetry of $O(n-1)$ and the well organized formula for the potential functions will greatly facilitate the next stage of analytic study of many body problems.

In concluding this foundational paper on the kinematic geometry of n-body systems, let us mention here a few concrete problems in celestial and quantum mechanics that the geometric foundation of this paper will provide an advantageous framework to start with.

7.1. The Problem of Central Configurations and Collisions

Let U be the Newtonian potential function of an n-body system with a given mass distribution. It is, of course, $SO(3)$ invariant and hence can be considered as a function defined on the orbit space $\overline{M}_n = M_n/SO(3)$. The configuration of total collision is the natural base point and the distance between a given configuration to that base point is given by the square root of its moment of inertia, i.e., $\rho = \sqrt{I}$. The Newtonian potential function U is of homogeneous degree of -1 with respect to the above scaling parameter ρ.

Hence

$$U = \frac{1}{\rho} U^*, \quad U^* = U|M_n^* = \{p \in \overline{M}_m;\ \rho(p) = 1\}.$$

Definition 7.1. *A configuration is called central if its corresponding "shape" (i.e., the homothetic one with $\rho = 1$) is a critical point of U^*.*

Example. In the beginning case of $n = 3$, U^* has four critical points, namely, the shape of regular triangle and the three colinear central configuration determined by Euler in a paper of 1767 (see [2]).

In a paper of Sundman[6], he proves that the shapes of a three-body system must approach one of the above four shapes as a limit when it is heading to a total collision. Such a result can be generalized to total collisions of n-body systems and this demonstrates the importance of the problem of central configurations.

7.2. The reduction of the Schröding's Equation of an n-Body System from the Level of M_n to the Level of $\overline{M}_n$

The Schrödinger's equation of a given n-body system in quantum mechanics is usually written as follows, namely

$$-\frac{\hbar^2}{2} \sum_{j=1}^{n} \frac{1}{\mu_j} \Delta_j \psi + U\psi = E\psi, \tag{7.1}$$

where $\{\mu_j;\ 1 \leq j \leq n\}$ are the individual masses and Δ_j is the Laplace operator with respect to the Cartesian Coordinates of the j-th particle. Using the center of mass reduction and the Jacobi metric on M_n, the above Schrödinger's equation can be rewritten as

$$-\frac{\hbar^2}{2\mu} \Delta\psi + U\psi = E\psi, \tag{7.1'}$$

where μ is the total mass and Δ is the Laplace operator on M_n with respect to the kinematic metric. The left-hand side of (7.1) is naturally an $SO(3)$-invariant (linear) differential operator, and this is the origin of angular momentum conservation in quantum mechanics. One way of maximizing the use of the $SO(3)$-invariance property of a given PDE is to achieve a suitable reduction to some corresponding PDE's solely defined at the orbit space level if such a reduction is, at all, possible. In the case of the 3-body problem, such a reduction of Schrödinger's equation to PDE's solely in terms of triangular parameters has been worked out recently the author[3,4], in which the use of the canonical coordinate system plays an important role. Actually, the canonical coordiate system of this paper is exactly the generalization of the coordinate system $(\mathbf{x}, \mathbf{y}) = (\xi_1\xi_2\xi_3; \eta_1\eta_2\eta_3)$ used in [3,4]. Such a coordinate system greatly facilitates the "equivariant-harmonic-analysis" on $(SO(3), M_3)$ thus enabling us to work out the $SO(3)$-reduction of the Schrödinger's equation of 3-body systems. Therefore, one of the natural applications of the canonical coordinate system of this paper will be to extened the $SO(3)$-reduction of the Schrödinger's equation to the general case of n-body systems by the same kind of equivariant-harmonic-analysis on $(SO(3), M_n)$. This will be the topic of one of its sequels and it will constitute the next step along the journey of solveing the Schrödinger's equation for many-body problems.

7.3. The $O(n-1)$-Symmetry on $\overline{M}_n$ and Its Equivariant-Harmonic-Analysis

Let Δ (resp. $\overline{\Delta}$) be the Laplace operators on M_n (resp. $\overline{M}_n$) with respect to the kinematic

Riemannian metrics on M_n (resp. $\overline{M}_n$) and v be the volume function on $\overline{M}_n$ which records the 3-dimensional volume of the $SO(3)$-orbits. Then, one has the folowing formula relating the above two Laplacians of an $SO(3)$-invariant function f, namely

$$\Delta f = \overline{\Delta} f + \langle \overline{\nabla} f, \overline{\nabla} \ln v \rangle_{\overline{M}_n} \tag{7.2}$$

where $\overline{\nabla}$ is the gradient with respect to the kinematic metric in $\overline{M}_n$. In the special case of zero angular momentum, the wave function ψ is $SO(3)$-invariant and hence the above formula directly produces the reduced Schrödinger's equation, namely

$$-\frac{\hbar^2}{2\mu}(\overline{\Delta}\psi + \langle \overline{\nabla}\psi, \overline{\nabla} \ln v \rangle_{\overline{M}}) + U\psi = E\psi. \tag{7.3}$$

In the general case of non-zero angular monentum, the second order differential operator of (7.2) will again be the leading term of the reduced PDE's (see [3,4] for the case of $n = 3$). The $O(n-1)$-invariance of the above second order differential operator will again provide the key for achieving "variable separation" and thus solving its eigenvalue, eigenfunction problem explicity. This, of course, will be the third major step toward the journey of solving the Schrödinger's equation for many-body problems.

Anyhow, with the canonical coordinate system, the additional kinematic symmetry of $O(n-1)$ and the well fitting simple formula of r_{ij} and hence that of the potential function at hand, the journey toward a systematic solution of the Schrödinger's equation for the many-body problem has, indeed, a good beginning.

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