The metric properties of the reduced nuclear configuration space: Remarks

Zbigniew Zimpel*
Department of Chemistry, University of Saskatchewan, Saskatoon, Saskatchewan, Canada S7N 0W0

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A definition of the distance on the orbit spaces of topological groups acting continuously on metric spaces is applied to define some metric properties of the reduced nuclear configuration spaces. Straightforward proofs are given and a comparison with former results is carried out.

Let (E, ρ) be a metric space, i.e. a set E with a distance function ρ [1]. We assume that there is a topological group G acting continuously on E [1]. The result of the action of an element t of G on a point x of E is an element $t \cdot x$ of E.

Let E/G denote the space of orbits of G in E, i.e. the set of mutually disjoint subsets of E defined as

$$\mathrm{G} \cdot x = \{s \cdot x : s \in \mathrm{G}\}. \tag{1}$$

We assume that E/G is a Hausdorff space, for which it is sufficient and necessary that for every orbit $K \in \mathrm{E/G}$ the "rectangle" $\{(x, y) : x, y \in K\}$ is a closed subset of the product space $\mathrm{E} \times \mathrm{E}$. Then the orbits are closed subsets of E.

We assume that ρ is invariant with respect to the action of G, which means that for every $s \in \mathrm{G}$ and $x, y \in \mathrm{E}$ the distance function obeys the equation

$$\rho(s \cdot x, s \cdot y) = \rho(x, y). \tag{2}$$

Before showing how the above introduced definitions can be applied to the reduced nuclear configuration space, we shall quote two general results.

*Permanent address: Institute of Molecular Physics, Polish Academy of Sciences, Smoluchowskiego 17/19, 60-179 Poznan, Poland

PROPOSITION 1

The function d from the orbit space E/G in R_+ given by

$$d(K, L) = \inf\{\rho(x, y): x \in K, y \in L\} \tag{3}$$

defines a distance function on E/G.

PROPOSITION 2

For any $x \in K$ and $y \in L$,

$$d(K, L) = \inf\{\rho(s \cdot x, y): s \in G\} = \inf\{\rho(x, s \cdot y): s \in G\}. \tag{4}$$

The proofs of both propositions are given in the appendix.

Proposition 1 states that E/G can be given a distance function defined by eq. (3). This procedure was applied by Mezey to the case of the reduced nuclear configuration space, where $E = R^{3N}$ and G is the group generated by all proper rotations and translations. Our new proof of his result, based on proposition 2, is also included in the appendix to demonstrate the ease with which d can be shown to be a distance function.

Another possibility of defining a distance on the nuclear configuration space was suggested in our recent paper [3]. There, we chose a symmetry-related reference frame (for example, one defined by three axes of fourfold symmetry in the case of octahedral symmetry) in which positions of nuclei have to be considered. Hence, instead of having a reduced configuration space with isolated configurations of nuclei, we deal with a full configuration space in which it is important to know about orientation of configuration with respect to a particular reference frame. Next, we carry out permutations of identical nuclei, taking the orbit of this permutation group to be the actual configuration.

To be more specific, let the vectors $\boldsymbol{v} = (\boldsymbol{r}_1, \boldsymbol{r}_2, \ldots, \boldsymbol{r}_N)$ and $\boldsymbol{v}' = (\boldsymbol{r}'_1, \boldsymbol{r}'_2, \ldots, \boldsymbol{r}'_N)$ define two configurations $\overline{\boldsymbol{v}}$ and $\overline{\boldsymbol{v}}'$ of N identical nuclei. These configurations are orbits of the group G_{iso} generated by proper rotations and translations according to ref. [2] or of the symmetric group S^N of all permutations of identical nuclei according to ref. [3]. Then the distance between these two configurations can be defined either by eq. (3) or by eq. (4).

However, as was discussed in our previous work [3], we can also determine the notion of *essential symmetry* of nuclear configurations by optimizing the choice of the symmetry-related reference frame (for example, the choice of rotation axes or reflection planes) in order to minimize the distance between a given configuration and its image by a considered transformation. We have found that this distance is equal to the distance between the orbits of the group generated by proper rotations and translations, which naturally operates on the space of orbits of S^N. This is also equivalent to saying that the degree of essential asymmetry (or, more specifically, chirality) proposed in ref. [3] is based on the metric defined in ref. [2] for the reduced nuclear configuration space with a minor modification, namely that the configurations resulting from permutations of identical nuclei are the same. In table 1, we summarize the metric properties of the nuclear configuration spaces defined by Mezey [2] and by us [3].

Table 1

Comparison of the metric properties of nuclear configuration spaces. G_{iso} denotes the group of isometries generated by translations T(3) and proper rotations SO(3) (the largest connected compact sub-group of the group of isometries) of R^{3N}. S^N is the symmetric group of all permutations of N nuclei, herein assumed to be identical. The action of G_{iso} and S^N on R^{3N} is defined as in ref. [3].

	Mezey's [2]	Ours [3]
initial configuration space E	R^{3N}	R^{3N}
distance function R^3	$\rho(x, y) = \left(\sum_{i=1}^{3} (x_i - y_i)^2 \right)^{1/2}$	$\rho(x, y) = \left(\sum_{i=1}^{3} (x_i - y_i)^2 \right)^{1/2}$
group G	$G_{iso} = SO(n)T(n)$	S^N
orbit space F = E/G	$F = R^{nN}/G_{iso}$	$F = R^{nN}/S^N$
distance function	defined by eq. (3)	defined by eq. (4)
relationship: orbit spaces	F/S^N	F/G_{iso}
relationship: distance functions	eq. (3) or (4) applied to F/S^N	eq. (3) or (4) applied to F/G_{iso}

For an arbitrary dimension n of the Euclidean space ($n = 3$ in the case of nuclear configurations considered above) in which a configuration of particles must be studied, another conclusion can be drawn from the above discussion, namely that taking an appropriate symmetry-related reference system as described in ref. [3] we can find a natural representation for each orbit of R^{nN}/G_{iso} by a point in R^{nN}. This can be achieved by choosing a system for which the degree of asymmetry, e.g. a declination from the octahedral symmetry, attains its minimal value. The actual reduction of the number of independent variables (from nN to $n(n-1)/2 + (N-n)n$ for $N \geq n$) then results from the number of constraint conditions (equal to $n + n(n-1)/2$ or less down to n for the determination of the origin of a coordinate system) they must obey. This approach can be very useful for computational purposes.

Appendix

Proof of proposition 2

Let two arbitrary points $x \in K$ and $y \in L$ be given. Thus, we have

$$
\begin{aligned}
d(K,L) &= \inf\{\rho(x,y):\ x \in K \ \text{and}\ y \in L\} = \inf\{\rho(s\cdot x, t\cdot y):\ s,t \in \mathrm{G}\} \\
&= \inf\{\rho((t^{-1}s)\cdot x, y):\ s,t \in \mathrm{G}\} = \inf\{\rho(s\cdot x, y):\ s \in \mathrm{G}\} \\
&= \inf\{\rho(x, s^{-1}\cdot y):\ s \in \mathrm{G}\} = \inf\{\rho(x, s\cdot y):\ s \in \mathrm{G}\}. \qquad \square
\end{aligned}
$$

Proof of proposition 1

Using the equivalence of definitions (3) and (4), it is easy to show that d is a distance function. The condition $d(K, K) = 0$ is obviously fulfilled. Let K and L be two orbits of E/G such that $d(K, L) = 0$. Let $x \in K$ and $y \in L$ be two arbitrary points within each orbit. Thus, the equation

$$0 = d(K, L) = \inf\{\rho(s\cdot x, y): s \in \mathrm{G}\}$$

implies that there is a sequence $(s_n)_{n\geq 1} \subset \mathrm{G}$ such that the sequence $\rho_n = \rho(s_n \cdot x, y)$ converges to 0. This is equivalent to saying that the sequence $(s_n \cdot x)_{n\geq 1} \subset K$ converges to $y \in L$ in E, However, since K and L are closed in E, this is possible if and only if $K = L$.

Now, let K, L and M be three orbits of E/G, and let $x \in K$, $y \in L$ and $z \in M$ be three arbitrary points of these orbits. Thus, we obtain

$$
\begin{aligned}
d(K,M) &= \inf\{\rho(s\cdot x, z):\ s \in \mathrm{G}\} = \inf\{\rho(s\cdot x, t\cdot z):\ s,t \in \mathrm{G}\} \\
&\leq \inf\{\rho(s\cdot x, y) + \rho(y, t\cdot z):\ s,t \in \mathrm{G}\} \\
&= \inf\{\rho(s\cdot x, y):\ s \in \mathrm{G}\} + \inf\{\rho(y, t\cdot z):\ t \in \mathrm{G}\} \\
&= d(K,L) + d(L,M),
\end{aligned}
$$

which proves the triangle inequality. Since the last condition, namely

$$d(K, L) = d(L, K) \ \text{for any}\ L, K \in \mathrm{E/G},$$

is trivially satisfied, we conclude that d is a distance function. □

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