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# Dynamical distance as a semi-metric on nuclear configuration space

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**Abstract.** In this paper, we introduce the concept of dynamical distance on a nuclear configuration space. We partition the nuclear configuration space into disjoint classes. This classification coincides with the classical partitioning of molecular systems via the concept of conjugacy of dynamical systems. It gives a quantitative criterion to distinguish different molecular structures.



**Keywords:** Dynamical distance, molecular structur, nuclear configuration, QTAIM.

**2010 AMS Subject Classification**: 97M60.

## 1. Introduction

Collard and Hall [10] introduced the foundations of topological analysis (abbreviated in TA) of one-electron charge densities and its mathematical foundations was reviewed in [2, 3, 18]. Also, TA was considered as an effective tool in modern computational chemistry [4, 5, 24].

The mathematical framework of TA is not limited to one-electron charge densities, since it is applied to other scaler functions, such as the nuclear potential energy field [25], the virial field [13], and the Laplacian of charge density [6, 7, 20]. TA of the potential energy hyper-surfaces was studied by Collard and Hall and then followed by Mezey [15, 16].

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Within this paper, the quantum theory of atoms in molecules (QTAIM) is considered as a method for TA. The TA of one-electron charge densities, within QTAIM is initiated by considering the gradient system

$$\frac{\partial \xi_x}{\partial t}(r,t) = \nabla \rho_x(\xi_x(r,t))$$

where $\nabla \rho_x$ is the gradient of one-electron charge density in a nuclear configuration $x$. Then one finds the critical points of $\rho_x$, i.e., the solution of the equation $\nabla \rho_x(z) = 0$. Finally, based on the spectrum of the Hessian matrix of $\rho_x$, the critical points of $\rho_x$ are classified.

Since the dynamical behaviour of the gradient system corresponding to the vector field $\nabla \rho_x$ is completely determined by the spectrum of the Hessian matrix of $\rho_x$, the nuclear configuration space may be classified based on TA above.

This paper is an attempt to classify the nuclear configuration space in a quantitative approach. More precisely, we are going to introduce a semi-metric, namely *dynamical distance*, on the nuclear configuration space $\Omega$ which, some how, measures how far the dynamical behaviour of the gradient systems given by $\nabla \rho_x$ and $\nabla \rho_y$ are. It results in a distance on the nuclear configuration space which, exactly, gives the same classification of nuclear configuration space, as in [17].

## 2. The nature of the problem

Structural stability of dynamical systems is one of the most fundamental concepts for researchers in different areas of science [26]. In particular, it may be applied to give an explicit definition of nuclear structure. For a molecular system, there exist different nuclear geometries $x$ or equivalently different electron charge densities $\rho_x$ where $x$ arises from Born-Oppenheimer approximation [8]. So, we have a correspondence $x \mapsto \rho_x$ between the points of nuclear configuration space and the family of electron charge densities. So, one may assign a gradient dynamical system $\xi_x$ to any point $x$ of the nuclear configuration space as follows:

$$\begin{aligned} x \mapsto \text{charge density } \rho_x \mapsto \text{gradient vector field } \nabla \rho_x \\ \mapsto \text{corresponding dynamical system } \xi_x. \end{aligned} \tag{1}$$

Therefore, we have the following equivalence relation on nuclear configuration space:

$$x \sim y \iff \text{the dynamical systems } \xi_x \text{ and } \xi_y \text{ are conjugate.}$$

This equivalence relation classifies the nuclear configuration space into equivalence classes $[x]$. Each of the equivalence classes $[x]$ corresponds to a molecular structure. Each open class $[x]$ is correspondent to a structural stable class. Catastrophic properties are appeared when the class $[x]$ is not open [21]. Integration on each equivalence class results in a type of information content of molecular structures [22].

The previous discussion gives a qualitative approach to partition the nuclear configuration space and therefore, to the concept of molecular structure.

A significant question concerning these equivalence classes is: Can one give a quantitative approach to partition the nuclear configuration space, resulting in the same equivalence classes?

In this paper, we show that the answer to the previous question is affirmative. We will extract the equivalence classes $[x]$ by defining a semi-metric on the configuration space $\Omega$.

## 3. Mathematical prerequisities

In this section, we provide the mathematical prerequisities which we need in the proceeding of the paper. First, we discuss some primary facts on linear algebra and then we make a short discussion on dynamical system and linearization.

### 3.1 *Linear algebra*

The linearity is a property which simplifies the study of dynamical systems. So, the linearization of a dynamical system is an important method for tracking the dynamical properties of a system. It leads to the study of matrices and their eigenvalues. In this section, we present some introductory facts about matrices.

Let $A$ be a square matrix with real arrays. Let $\lambda$ be an eigenvalue of $A$. The multiplicity of $\lambda$, as a root of the characteristic polynomial $\det(A-\lambda I)=0$, is denoted by $m_\lambda$, and the nullity of $A-\lambda I$ is given by $n_\lambda := \dim N(A-\lambda I)$. We also write $\tau_\lambda$ for the sign of $\lambda$, i. e.,

$$\tau_\lambda = \begin{cases} -1 \text{ if } \lambda < 0 \\ 0 \text{ if } \lambda = 0 \\ 1 \text{ if } \lambda > 0 \end{cases}$$

A Jordan $\lambda$-block is a square matrix in one of the following forms:

$$\begin{bmatrix}\lambda\end{bmatrix}, \quad \begin{bmatrix}\lambda & 1 \\ 0 & \lambda\end{bmatrix}, \quad \begin{bmatrix}\lambda & 1 & 0 \\ 0 & \lambda & 1 \\ 0 & 0 & \lambda\end{bmatrix}$$

and so on.

It is known that, every square matrix $A$ is similar to a block diagonal matrix, consisting entirely of such blocks, which is called the Jordan form of $A$. The following facts are known: [11]

**Fact 1:** If $\lambda$ is an eigenvalue of multiplicity $m_\lambda$, then $m_\lambda$ must appear $m_\lambda$ times on the diagonal of the Jordan form.

**Fact 2:** $n_\lambda = \dim N(A-\lambda I)$ is the number of Jordan $\lambda$-blocks.

**Definition 3.1** Let $A$ and $B$ be two $n\times n$ matrices with real eigenvalues. Let $\lambda_1,...,\lambda_n$ and $\mu_1,...,\mu_n$ be the eigenvalues of $A$ and $B$ respectively. Then $A$ and $B$ are said to be *equivalent* if there is a permutation $\sigma:\{1,2,...,n\}\to\{1,2,...,n\}$ such that

$$m_{\lambda_j} = m_{\mu_{\sigma(j)}}, \quad n_{\lambda_j} = n_{\mu_{\sigma(j)}}, \quad \tau_{\lambda_j} = \tau_{\mu_{\sigma(j)}}$$

for all $j\in\{1,2,...,n\}$.

Clearly, any two similar matrices are equivalent.

### 3.2 *Dynamical systems*

In section 4 we use some general techniques of dynamical systems to classify the nuclear configuration space. we discuss the minimum material which is needed in the sequel.

#### *3.2.1 The general theory*

In this part, we recall the minimum necessary facts of the theory of dynamical systems for TA. Since our discussion is limited to $\mathbb{R}^3$, we only consider dynamical systems on $\mathbb{R}^3$, however, more general discussions may be found in the classical contexts [1, 9, 19, 23].

Consider a system of ordinary differential equations

$$\frac{dx}{dt} = F(x) \tag{2}$$

where $x : \mathbb{R} \to \mathbb{R}^3$ and $F : \mathbb{R}^3 \to \mathbb{R}^3$ are smooth functions. The solution of the system of differential equations (2) results in the flow $\phi : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$ satisfying the following conditions:

$$\frac{\partial \phi}{\partial t}(x,t) = F(\phi(x,t)), \quad \phi(x,0) = 0, \quad \phi(x,t+s) = \phi(\phi(x,t),s) \tag{3}$$

for all $x \in \mathbb{R}^3$ and $t, s \in \mathbb{R}$.

Two dynamical systems $\phi, \psi : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$ are said to be conjugate, if there is a diffeomorphism (A differentiable map with differentiable inverse) $h : \mathbb{R}^3 \to \mathbb{R}^3$ such that

$$h(\phi(x,s)) = \psi(h(x),s)$$

for all $x \in \mathbb{R}^3$ and $t \in \mathbb{R}$. Indeed, two conjugate dynamical systems have the same dynamical behaviour.

Based on the concept of conjugacy, it is possible to define an equivalence relation on a family of dynamical systems. It classifies the family of dynamical systems into equivalence classes. It results in a mathematical definition of structural stability and instability for a dynamical system.

#### *3.2.2 Linear systems and linearization*

Suppose that $A$ is a $3 \times 3$ matrix. If we set $F(X) = Ax$, in equation (2), then we get a linear system of differential equations

$$\frac{dx}{dt} = Ax. \tag{4}$$

If $J$ is the Jordan form of $A$ then the dynamical system associated to (4) is conjugate to the linear system given by

$$\frac{dx}{dt} = Jx. \tag{5}$$

So, the dynamics of the solution of (5), and therefore (4), is completely determined by the eigenvalues of $A$.

Consider the system

$$\frac{dx}{dt} = F(x)$$

and suppose that $F(x_0) = 0$. Let $DF_{x_0}$ denotes the Jaccobian matrix of $F$ evaluated at $x_0$. then the linear system of differential equations

$$\frac{dy}{dt} = DF_{x_0} y \tag{6}$$

is called the linearalized system near $x_0$. Note that, if $x_0 = 0$, the linearalized system is obtained by simply dropping all of the nonlinear terms in $F$.

If $x_0$ is an equilibrium point of a linear system (4), then the behaviour of the dynamical system corresponding to (4), in a neighbourhood of $x_0$ is completely determined by the eigenvalues of $A$ in (4), i.e., by the number of the eigenvalues, their multiplicity and their sign.

The following theorem states that solutions of nonlinear systems near equilibrium points resemble those of their linear parts only in the case where the linearized system is hyperbolic; that is, when neither of the eigenvalues of the system has zero real part [12].

**Theorem 3.2** (The Linearization Theorem) Suppose the n-dimensional nonlinear system $\frac{dx}{dt} = F(x)$ has an equilibrium point at $x_0$ that is hyperbolic. Then the nonlinear flow is conjugate to the flow of the linearized system in a neighborhood of $x_0$.

Applying Theorem 3.2 and considering the fact that, the dynamical behaviour of any linear system such as (4) is completely determined by eigenvalues of $A$, two nonlinear systems $\frac{dx}{dt} = F(x)$ and $\frac{dx}{dt} = G(x)$, with hyperbolic equilibrium points, are conjugate if there is a correspondence $x_0 \mapsto x_0^*$ between their equilibrium points such that the linearalized systems $\frac{dx}{dt} = DF_{x_0} x$ and $\frac{dx}{dt} = DG_{x_0^*} x$ have similar behaviour, in the sense that, $DF_{x_0}$ and $DG_{x_0^*}$ are two equivalent matrices.

The following theorem is useful since we work with gradient systems [12].

**Theorem 3.3** Let $f : \mathbb{R}^3 \to \mathbb{R}$ be a smooth scaler field. For a gradient system $\frac{dx}{dt} = \nabla f(x)$, the linearized system at any equilibrium point has only real eigenvalues.

Note that, positive eigenvalues lead to the unstable manifolds and the negative eigenvalues lead to the stable manifolds [14, 21].

## 4. Dynamical distance

Suppose that $M$ is a molecule and $x$ the corresponding nuclear configuration (molecule geometry). Then the wave function of this molecule is denoted by $\Psi = \Psi(r; x)$, where $r$ stands for the collection of electronic variables and $x$ is to emphasize the parametric dependence of the wave function to the nuclear coordinates. Therefore, the one-electron charge density $\rho_x$, and so, the corresponding gradient vector field $\nabla\rho_x$ are also dependent parametrically on the nuclear configuration $x$. Bader and coworkers [3, 10] introduced the differential equation

$$\frac{dr(s)}{ds} = \nabla\rho_x(r(s)) \tag{7}$$

which results in the dynamical system $\xi_x : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{R}^3$ satisfying

$$\xi_x(r, 0) = r, \qquad \frac{\partial \xi_x}{\partial t}(r, t) = \nabla\rho_x(\xi_x(r, t)) \tag{8}$$

for all $r \in \mathbb{R}^3$. Since for any point in the nuclear configuration space, there is a certain dynamical system, the equivalence relation "$\sim$" could be defined on the nuclear configuration space:

$$x \sim y \iff \text{the dynamical systems } \xi_x \text{ and } \xi_y \text{ are conjugate.}$$

Thus, the nuclear configuration space is classified into equivalence classes. Each equivalence class is denoted by $[x]$. The previous approach results in the definition of a molecular structure, stability and instability of molecular structures [3, 10].

In this section, we are going to define a map $j : \Omega \times \Omega \to [0, \infty)$ which generates the previous equivalence classes in a quantitative approach.

Note that, the equilibrium points of the dynamical system given by (8) (points $P$ where $\nabla\rho_x(P) = 0$) are divided into two parts:

Firstly, the points $P$ which the Hessian matrix $H = \nabla\nabla^T\rho_x$ is invertible, i.e., $\det H(P) \neq 0$. The critical points in this case are called non-degenerate, and the Hessian matrix $H(P) = \nabla\nabla^T\rho_x(P)$ is a hyperbolic matrix.

Secondly, the Hessian matrix $H(P) = \nabla\nabla^T\rho_x(P)$ is not invertible, i.e., $\det H(P) = 0$. In this case, the Hessian matrix $H(P) = \nabla\nabla^T\rho_x(P)$ possesses at least one null eigenvalue. The critical points, in this case, are called degenerate.

We assume that $M$ is a molecule with nuclear configurations so that all (a finite number) the critical points are non-degenerate. Note that, other cases, with infinite number of critical points, are very special and extremely rare [3].

Suppose that $x$ and $y$ are two nuclear configurations, and $\rho_x$ and $\rho_y$ are the corresponding one-electron charge densities. Let $P \in \nabla\rho_x^{-1}(\{0\})$ and $Q \in \nabla\rho_y^{-1}(\{0\})$. Let also $\nabla\nabla^T\rho_x(P)$ and $\nabla\nabla^T\rho_y(Q)$ be the Hessian matrices corresponding to $\rho_x$ and $\rho_y$, evaluated at $P$ and $Q$ respectively. Let $\lambda_1(P), \lambda_2(P), \lambda_3(P)$ be the eigenvalues of $\nabla\nabla^T\rho_x(P)$ and $\mu_1(Q), \mu_2(Q), \mu_3(Q)$ be the eigenvalues of $\nabla\nabla^T\rho_y(Q)$. Note that, by Theorem 3.3, $\lambda_j(P)$ and $\mu_j(Q)$ $(j = 1, 2, 3)$ are real numbers. The *local dynamical distance* of $x$ and $y$ at $P$ and $Q$ is defined as follows:

$$\alpha_{(x,y)}(P, Q) := \min_{\sigma \in S_3} \left\{ \sum_{i=1}^{3} |m_{\lambda_i(P)} - m_{\mu_{\sigma(i)}(Q)}| + \sum_{i=1}^{3} |n_{\lambda_i(P)} - n_{\mu_{\sigma(i)}(Q)}| + \sum_{i=1}^{3} |\tau_{\lambda_i(P)} - \tau_{\mu_{\sigma(i)}(Q)}| \right\}$$

where $S_n$ is the collection of all permutations on $n$. Now, suppose that

$$\nabla\rho_x^{-1}(\{0\}) = \{P_1, P_2, ..., P_{l_x}\}$$

and

$$\nabla\rho_y^{-1}(\{0\}) = \{Q_1, Q_2, ..., Q_{l_y}\}.$$

The *dynamical distance* of $x$ and $y$ is defined as follows:

$$j(x, y) := \begin{cases} \min_{\delta \in S_l} \left\{ \sum_{j=1}^{l} \alpha_{(x,y)}(P_j, Q_{\delta(j)}) \right\} & \text{if } l_x = l_y = l \\ |l_x - l_y| & \text{if } l_x \neq l_y \end{cases}$$

Briefly, we have defined a map $j : \Omega \times \Omega \to [0, \infty)$ which assigns a non-negative integer to any two nuclear configurations. It, some how, measures how far are the dynamics generated by two nuclear configurations.

One may easily check the following properties:

(1) $j(x,x) = 0$ for all $x \in \Omega$.
(2) $j(x,y) = j(y,x)$ for all $x, y \in \Omega$.
(3) $j(x,z) \leqslant j(x,y) + j(y,z)$ for all $x, y, z \in \Omega$.

So, the dynamical distance $j : \Omega \times \Omega \to [0,\infty)$ is indeed a semi-metric on the nuclear configuration space. However, the following theorem states that $j$ is not a metric, but it partitions the nuclear configuration space just the same as [17].

**Theorem 4.1** For any two nuclear configurations $x$ and $y$ we have

$$j(x,y) = 0 \text{ if and only if } [x] = [y].$$

**Proof.** Suppose that $[x] = [y]$. Thus, the dynamical systems $\xi_x$ and $\xi_y$ are conjugate. In particular, $l_x = l_y = l$. Let $\{P_1, P_2, ..., P_l\}$ and $\{Q_1, Q_2, ..., Q_l\}$ be the critical points of $\nabla\rho_x$ and $\nabla\rho_y$ respectively. For $i \in \{1, 2, ..., l\}$, the nonlinear system

$$\frac{\partial \xi_x}{\partial t}(r,t) = \nabla\rho_x(\xi_x(r,t)) \tag{9}$$

is conjugate to the linear system

$$\frac{\partial \xi_x}{\partial t}(r,t) = \nabla\nabla^T\rho_x(P_i)\xi_x(r,t) \tag{10}$$

near the equilibrium point $P_i$. Similarly, the nonlinear system

$$\frac{\partial \xi_y}{\partial t}(r,t) = \nabla\rho_y(\xi_y(r,t)) \tag{11}$$

is conjugate to the linear system

$$\frac{\partial \xi_y}{\partial t}(r,t) = \nabla\nabla^T\rho_y(Q_i)\xi_y(r,t) \tag{12}$$

near the equilibrium point $Q_i$. So, there is a permutation $\delta \in S_l$ such that for any $i \in \{1, 2, ..., l\}$ the linear systems corresponding to the Hessian matrices $\nabla\nabla^T\rho_x(P_i)$ and $\nabla\nabla^T\rho_y(Q_{\delta(i)})$ are conjugate. Since the dynamic of any linear system is completely determined by the eigenvalues of its coefficient matrix then the Hessian matrices $\nabla\nabla^T\rho_x(P_i)$ and $\nabla\nabla^T\rho_y(Q_{\delta i})$ are equivalent. So, there is a permutation $\sigma \in S_3$ such that

$$m_{\lambda_j(P_i)} = m_{\mu_{\sigma(j)}(Q_{\delta(i)})}, \quad n_{\lambda_j(P_i)} = n_{\mu_{\sigma(j)}(Q_{\delta(i)})}, \quad \tau_{\lambda_j(P_i)} = \tau_{\mu_{\sigma(j)}(Q_{\delta(i)})}$$

for all $j \in \{1, 2, 3\}$. Therefore, $\alpha_{(x,y)}(P_i, Q_{\delta(i)}) = 0$ for all $i \in \{1, 2, ..., l\}$. This easily results in $j(x,y) = 0$.

Conversely, let $j(x,y) = 0$. By the definition of $j$, $l_x = l_y = l$ and

$$\min_{\delta \in S_l} \left\{ \sum_{j=1}^{l} \alpha_{(x,y)}(P_j, Q_{\delta(j)}) \right\} = 0.$$

Hence, there is a permutation $\delta \in S_l$ such that

$$\sum_{j=1}^{l} \alpha_{(x,y)}(P_j, Q_{\delta(j)}) = 0,$$

so $\alpha_{(x,y)}(P_j, Q_{\delta(j)}) = 0$ for all $j \in \{1, 2, ..., l\}$. Consequently, for any $j \in \{1, 2, ..., l\}$ there exists a permutation $\sigma \in S_3$ such that

$$m_{\lambda_i(P_j)} = m_{\mu_{\sigma(i)}(Q_{\delta(j)})}, \quad n_{\lambda_i(P_j)} = n_{\mu_{\sigma(i)}(Q_{\delta(j)})}, \quad \tau_{\lambda_i(P_j)} = \tau_{\mu_{\sigma(i)}(Q_{\delta(j)})}.$$

Therefore $\nabla\nabla^T\rho_x(P_j)$ and $\nabla\nabla^T\rho_y(Q_{\delta(j)})$ are equivalent matrices, for all $j \in \{1, 2, ..., l\}$. So, the corresponding linear systems are conjugate. By Theorem 3.2 the linear system

$$\frac{\partial \xi_x}{\partial t}(r, t) = \nabla\nabla^T\rho_x(P_j)\xi_x(r, t) \tag{13}$$

is conjugate to the nonlinear system (9) near the equilibrium point $P_j$ ($j \in \{1, 2, ..., l\}$). Similarly, the linear system

$$\frac{\partial \xi_y}{\partial t}(r, t) = \nabla\nabla^T\rho_y(Q_{\delta(j)})\xi_y(r, t) \tag{14}$$

is conjugate to the nonlinear system (11) near the equilibrium point $Q_{\delta(j)}$ where, $j \in \{1, 2, ..., l\}$. Consequently, the systems $\xi_x$ and $\xi_y$ are conjugate, therefore $[x] = [y]$. ■

## 5. Summary and discussion

In this paper, we introduced the concept of dynamical distance on nuclear configuration space. It is a semi-metric which defines a distance between any two nuclear configurations. The distance between two nuclear configurations $x$ and $y$ is zero if and only if the corresponding dynamical systems $\xi_x$ and $\xi_y$ have the same dynamical behaviour. In other words, the distance between two nuclear configurations is zero if and only if they have the same molecular structure. In this account, one may partition the nuclear configuration space $\Omega$ by defining the following equivalence relation:

$$x \sim_* y \text{ if and only if } j(x, y) = 0.$$

If we denote the equivalence class of $x$ by $[x]_*$ then Theorem 4.1 states that $[x] = [x]_*$ where $[x]$ is the equivalence class given by the equivalence relation [17]

$$x \sim y \iff \text{the dynamical systems } \xi_x \text{ and } \xi_y \text{ are conjugate.}$$

This results in a quantitative approach to partition the nuclear configuration space.

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