BULETINUL INSTITUTULUI POLITEHNIC DIN IAŞI

Volumul 64 (68)
Numărul 2

Secția
MATEMATICĂ
MECANICĂ TEORETICĂ
FIZICĂ

2018 **Editura POLITEHNIUM**

BULETINUL INSTITUTULUI POLITEHNIC DIN IAŞI
PUBLISHED BY
"GHEORGHE ASACHI" TECHNICAL UNIVERSITY OF IAŞI
Editorial Office: Bd. D. Mangeron 63, 700050, Iaşi, ROMANIA
Tel. 40-232-278683; Fax: 40-232-211667; e-mail: buletin-ipi@tuiasi.ro

BULETINUL INSTITUTULUI POLITEHNIC DIN IAŞI
BULLETIN OF THE POLYTECHNIC INSTITUTE OF IAŞI
Volumul 64 (68), Numărul 2 2018

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BULLETIN OF THE POLYTECHNIC INSTITUTE OF IAŞI
Volume 64 (68), Number 2 2018

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VARIANTS OF ATOMICITY AND SOME PHYSICAL APPLICATIONS

BY

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Received: April 10, 2018
Accepted for publication: May 18, 2018

Abstract. In this paper, some results concerning various forms of atomicity are given from the Quantum Measure Theory mathematical perspective and several physical applications are provided. Precisely, the mathematical concept of minimal atomicity is extended, and, based on the remark that Quantum Mechanics is a particular case of Fractal Mechanics for a specified scale resolution, the concept of fractal atomicity (and, particularly, fractal minimal atomicity) is introduced. Some of their mathematical properties are also given.

Keywords: Atom; Pseudo-atom; Minimal atom; Fractal atom; Null-additive set (multi)function.

1. Introduction

Measure Theory concerns with assigning a notion of size to sets. In the last years, non-additive measures theory was given an increasing interest due to its various applications in a wide range of areas. It is used to describe situations concerning conflicts or cooperations among intelligent rational players, giving an appropriate mathematical framework to predict the outcome of the process. Precisely, theories dealing with (pseudo)atoms and monotonicity are used in

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statistics, game theory, probabilities, artificial intelligence. The notion of non-atomicity for set (multi)functions plays a key role in measure theory and its applications and extensions. Even just replacing-additivity with finite additivity for measures requires some stronger non-atomicity property for the same conclusion to hold.

(Non)atomic measures and purely atomic measures have been investigated (in different variants) due to their special form and their special properties, *e.g.* (Chiţescu, 1975, 2001; Cavaliere and Ventriglia, 2014; Gavriluţ and Agop, 2016; Gavriluţ and Croitoru, 2008, 2009, 2010; Gavriluţ, 2010, 2011, 2012; Gavriluţ *et al*., 2015; Khare and Singh, 2008; Li *et al.*, 2014, 2015; Pap, 1994, 1995, 2002; Pap *et al.* 2016; Rao and Rao, 1983; Suzuki, 1991; Wu and Bo, 2007).

One important application of Measure Theory is in probability, where a measurable set is interpreted as an event and its measure as the probability that the event will occur. Since probability is an important notion in Quantum Mechanics, Measure Theory's techniques could be used to study quantum phenomena. Unfortunately, one of the foundational axioms of Measure Theory does not remain valid in its intuitive application to Quantum Mechanics.

Although classical measure theory imposes strict additivity conditions, a rich theory of non-additive measures developed. Precisely, modifications of traditional Measure Theory (Pap, 1994, 1995, 2002) led to Quantum Measure Theory (Gudder, 2009a, 2009b, 2010, 2011a, 2011b; Salgado, 2002; Sorkin, 1994, 1997, 2007; Surya and Waldlden, 2008). Practically, an extended notion of a measure has been introduced and its applications to the study of interference, probability, and space-time histories in Quantum Mechanics have been discussed (Schweizer and Sklar, 1983).

Quantum Measure Theory is a generalization of Quantum Theory where physical predictions are computed from a matrix known as a decoherence functional. Introduced by (Sorkin, 1994, 1997, 2007), quantum measures help us to describe Quantum Mechanics and its applications to Quantum Gravity and Cosmology (Hartle, 1990). Quantum Measure Theory indicates a wide variety of applications, its mathematical structure being used in the standard quantum formalism.

Despite the continuous efforts of numerous scientists, reconciling General Relativity with Quantum Theory remains one of the most important open problems in Physics. The framework of General Relativity suggests that one promising approach to such unification will be by means of a reformulation of Quantum Theory in terms of histories rather than states. Following this idea, (Sorkin, 1994, 1997, 2007), has proposed a history-based framework, which can unify standard Quantum Mechanics as well as physical theories beyond the quantum formalism.

In such framework, Schrödinger's equation from Quantum Mechanics can be identified with a particular type of geodesic of the fractal space. In

consequence, fundamental concepts of Quantum Mechanics can be extended to similar concepts, but on fractal manifolds. The aim of this paper is to provide the mathematical-physical framework that is necessary to extend some of these concepts. Precisely, we extend the concept of atoms/pseudo-atoms to the concept of fractal minimal atom/fractal pseudo-atom, respectively. We also give characterizations from a mathematical viewpoint to these new concepts and we make explicit certain physical implications. The notion of a fractal minimal atom as a particular case of fractal atom is also discussed.

2. Towards Quantum Measure Theory by Means of Fractal Mechanics

The basic idea behind Quantum Measure Theory, or Generalized Quantum Mechanics, for that matter, is to provide a description of the world in terms of histories. A history is a classical description of the system under consideration for a given period of time, finite or infinite. If we are trying to describe a system of N particles, then a history will be given by N classical trajectories. If we are working with a field theory, then a history will correspond to the spatial configuration of the field as a function of time. In either case, Quantum Measure Theory tries to provide a way to describe the world through classical histories by extending the notion of probability theory which is clearly not rich enough to model our universe.

On the other hand, structures, self-structures etc. of the Nature can be assimilated to complex systems, taking into account both their functionality, as well as their structure (Mitchell, 2009; Nottale, 2011). The models commonly used to study the dynamics of complex systems are based on the assumption, otherwise unjustified, of the differentiability of the physical quantities that describe it, such as density, momentum, energy etc. (for mathematical models and for applications, see (Mercheş and Agop, 2015; Nottale, 2011).

The success of differentiable models must be understood sequentially, *i.e.* on domains large enough that differentiability and integrability are valid. But differential method fails when facing the physical reality, with non-differentiable or non-integral physical dynamics, such as instabilities in the case of dynamics of complex systems, instabilities that can generate both chaos and patterns.

In order to describe such dynamics of complex systems, but still remaining tributary to a differential hypothesis, it is necessary to introduce, in an explicit manner, the scale resolution in the expressions of the physical variables that describe these dynamics and, implicitly, in the fundamental equations of "evolution" (for example, density, momentum, energy equations etc.). This means that any dynamic variable, dependent, in a classical meaning, on both spatial coordinates and time (Michel and Thomas, 2012; Mitchell, 2009), becomes, in this new context, dependent also on the resolution scale.

In other words, instead of working with a dynamic variable, described through a strictly non-differentiable mathematical function, we will just work with different approximations of that function, derived through its averaging at different resolution scales. Consequently, any dynamic variable acts as the limit of a functions family, the function being non-differentiable for a null resolution scale and differentiable for a non-zero resolution scale.

This approach, well adapted for applications in the field of dynamics of complex systems, where any real determination is conducted at a finite resolution scale, clearly implies the development both of a new geometric structure and of a physical theory (applied to dynamics of complex systems) for which the motion laws, invariant to spatial and temporal coordinates transformations, are integrated with scale laws, invariant at scale transformations.

Such a theory that includes the geometric structure based on the above presented assumptions was developed in the Scale Relativity Theory (Nottale, 2011) and more recently in the Scale Relativity Theory with an arbitrary constant fractal dimension (Mercheş and Agop, 2015). Both theories define the "fractal physics models" class (Mercheş and Agop, 2015; Nottale, 2011).

Various theoretical aspects and applications of the Scale Relativity Theory with an arbitrary constant fractal dimension in the field of physics are presented in (Mercheş and Agop, 2015; Nottale, 2011). In this model, if we assume that the complexity of interactions in the dynamics of complex systems is replaced by non-differentiability, then the motions constrained on continuous, but differentiable curves in an Euclidean space are replaced with free motions, without any constrains, on continuous, but non-differentiable curves (fractal curves) in a fractal space. In other words, for time resolution scale that prove to be large when compared with the inverse of the highest Lyapunov exponent (Mandelbrot, 1983), the deterministic trajectories are replaced by a collection of potential routes, so that the concept of "definite positions" is substituted by that of an ensemble of positions having a definite probability density (Mandelbrot, 1983; Mercheş and Agop, 2015; Nottale, 2011).

In consequence, the motion curves have double identity: both geodesics of the fractal space and streamlines of a fractal fluid, whose entities (the structural units of the complex system) are substituted with the geodesics themselves so that any external constrains are interpreted as a selection of geodesics by means of measuring device.

Since in such conjecture the Quantum Mechanics becomes a particular case of Fractal Mechanics, then Quantum Measure Theory could become, in our opinion, a particular type of a Fractal Measure Theory.

3. Minimal Atoms

Let T be an abstract nonvoid set, $\mathcal{C}$ a ring of subsets of T, X a Banach space, $\mathcal{P}_f(X)$ the family of all nonvoid closed subsets of X and $\mu : \mathcal{C} \to \mathcal{P}_f(X)$ an arbitrary set multifunction which satisfies the condition $\mu(\emptyset) = \{0\}$.

By $|\mu|$, defined on $\mathcal{C}$ and taking values in $[0,\infty]$, we mean the set function defined for every $A \in \mathcal{C}$ by $|\mu(A)| = h(\mu(A),\{0\})$, where h is the Hausdorff-Pompeiu pseudo-metric (Gavriluţ, 2012).

Definition 3.1 I) We say that μ is:

(i) *monotone* with respect to the inclusion of sets if $\mu(A) \subseteq \mu(B)$, for every $A, B \in \mathcal{C}$, with $A \subseteq B$;

(ii) *null-additive* if $\mu(A \cup B) = \mu(A)$, for every $A, B \in \mathcal{C}$, with $\mu(B) = 0$;

(iii) *null-null-additive* if $\mu(A \cup B) = \{0\}$, for every $A, B \in \mathcal{C}$, with $\mu(A) = \mu(B) = \{0\}$.

II) We say that a set $A \in \mathcal{C}$ is:

(i) *a minimal atom of* μ if $\mu(A) \supseteq \{0\}$, $\mu(A) \neq \{0\}$ and for every $B \in \mathcal{C}, B \subseteq A$, we have either $\mu(B) = \{0\}$ or $A = B$;

(ii) (Gavriluţ, 2010, 2011, 2012; Gavriluţ and Croitoru, 2008, 2009, 2010) *an atom of* μ if $\mu(A) \supseteq \{0\}$, $\mu(A) \neq \{0\}$ and for every $B \in \mathcal{C}, B \subseteq A$, we have either $\mu(B) = \{0\}$ or $\mu(A \setminus B) = \{0\}$;

(iii) (Gavriluţ, 2010, 2011, 2012; Gavriluţ and Croitoru, 2008, 2009, 2010) *a pseudo-atom of* μ if $\mu(A) \supseteq \{0\}$, $\mu(A) \neq \{0\}$ and for every $B \in \mathcal{C}, B \subseteq A$, we have either $\mu(B) = \{0\}$ or $\mu(A) = \mu(B)$.

Obviously, there exist atoms which are not minimal atoms.

We denote by A the collection of all atoms of μ and by MA the collection of all minimal atoms of μ. In what follows, suppose that μ is *monotone*.

Remark 3.2 (i) Any minimal atom is also an atom (and a pseudo-atom), so,

$\mathcal{MA} = \{A \in \mathcal{C}; \mu(A) \supseteq \{0\}, \quad \mu(A) \neq \{0\}$ and for every $B \in \mathcal{C}, B \subseteq A, B \neq A$ we have $\mu(B) = \{0\}\} \subseteq$

$\subseteq \mathcal{A} = \{A \in \mathcal{C}; \mu(A) \supseteq \{0\}, \mu(A) \neq \{0\}$ and for every $B \in \mathcal{C}, B \subseteq A$ we have either $\mu(B) = \{0\}$ or $\mu(A \setminus B) = \{0\}\}$;

(ii) If, moreover, μ is null-additive, then any atom of μ is also a pseudo-atom;

(iii) If A is a minimal atom of μ, then for every $B \in \mathsf{C}, B \subseteq A, B \neq A$ we have $\mu(B) \supseteq \{0\}, \mu(B) \neq \{0\}$;

(iv) If $m : \mathsf{C} \to [0, \infty)$ is monotone, $m(\varnothing) = 0$ and $\mu : \mathsf{C} \to \mathsf{P}_f(\mathsf{R})$, $\mu(A) = [0, m(A)]$, for every $A \in \mathsf{C}$, then a set $A \in \mathsf{C}$ is an atom / pseudo-atom / minimal atom of μ if and only if the same is A for m in the sense of (Mesiar *et al*., 2017; Ouyang *et al*., 2015).

μ is called *the set multifunction induced by the set function* m.

In consequence, one can have different examples concerning minimal atoms with respect to the set multifunction induced by a set function, taking as starting point the examples given in (Mesiar *et al*., 2017; Ouyang *et al*., 2015).

Proposition 3.3 *If* $\mu : \mathsf{C} \to \mathsf{P}_f(X)$ *is null-null-additive and* $A, B \in \mathsf{C}$ *are two different minimal atoms of* μ, *then* $A \cap B = \varnothing$.

Proof. Suppose that, on the contrary, there exist two non-disjoint, different minimal atoms $A, B \in \mathsf{C}$ of μ. Since $A \setminus (A \cap B) = A \setminus B \subseteq A$ and $A \cap B \subseteq B$, then $[\mu(A \setminus B) = \{0\}$ or $A \setminus B = A]$ and $[\mu(A \cap B) = \{0\}$ or $A \cap B = B]$.

(i) If $\mu(A \setminus B) = \{0\}, \mu(A \cap B) = \{0\}$, since μ is null-null-additive, we get that $\mu(A) = \{0\}$, a contradiction.

(ii) If $A \setminus B = A$, then $A \cap B = \varnothing$, a contradiction.

(iii) If $\mu(A \setminus B) = \{0\}$ and $A \cap B = B$, then $B \subseteq A$, so $\mu(B) = \{0\}$ (or $B = A$, which is false), so again by the null-null-additivity of μ, we have $\mu(A) = \{0\}$, a contradiction.

Evidently, if $A \in \mathsf{C}$ is a minimal atom of μ, it can not exist another different minimal atom $A_1 \in \mathsf{C}$ of μ so that $A_1 \subset A$.

Proposition 3.4 *(i) If* T *is finite, then for every* $A \in \mathsf{C}$, *with* $\mu(A) \supseteq \{0\}, \mu(A) \neq \{0\}$, *there exists* $B \in \mathsf{C}, B \subseteq A$, *which is a minimal atom of* μ.

(ii) If, moreover, A *is an atom of* μ *and* μ *is null-additive, then* $\mu(A) = \mu(B)$ *and the set* B *is unique.*

Proof. (i) Let us consider the collection of sets $\mathsf{M} = \{M \in \mathsf{C}, M \subseteq A, \mu(M) \supseteq \{0\}, \mu(M) \neq \{0\}\}$. Obviously, $\mathrm{M} \neq \varnothing$, since $A \in \mathsf{C}$. We remark that any minimal element of M is a minimal atom of μ. Indeed, let $M \in \mathrm{M}$ be a minimal element of M. Evidently, there can not exist $D \in \mathrm{M}$ so that $D \subseteq M$ and $D \neq M$ (*).

Since $M \in \mathrm{M}$, then $M \in \mathsf{C}, M \subseteq A, \mu(M) \supseteq \{0\}, \mu(M) \neq \{0\}$.

We demonstrate that M is a minimal atom of μ . Indeed, for any $S \subseteq M$, $S \in \mathsf{C}$, we have either $\mu(S) = \{0\}$ or $\mu(S) \supseteq \{0\}, \mu(S) \neq \{0\}$. In the latter case, we have either $S = M$ or $S \neq M$, which is in contradiction with $(*)$.

(ii) If on the contrary there are two different minimal atoms B_1 and B_2 of μ , then $\mu(A \setminus B_1) = \mu(A \setminus B_2) = \{0\}$, whence $\mu(A) = \{0\}$, a contradiction.

Proposition 3.5 (self-similarity of minimal atoms). *Any subset* $B \in \mathsf{C}$, *with* $\mu(B) \supseteq \{0\}, \mu(B) \neq \{0\}$ *of a minimal atom* $A \in \mathsf{C}$ *of* μ *is a minimal atom of* μ, *too.*

Proof. Let $A \in \mathsf{C}$ be a minimal atom of μ and consider any $B \in \mathsf{C}$, with $\mu(B) \supseteq \{0\}, \mu(B) \neq \{0\}$, $B \subseteq A$. We prove that B is a minimal atom of μ. Indeed, for any $C \in \mathsf{C}, C \subseteq B$, then $C \subseteq A$, so either $\mu(C) = \{0\}$ or $C = A$, whence $C = B$.

Example 3.6 (i) Suppose that $\mu_1, \mu_2 : \mathsf{C} \to \mathsf{P}_f(\mathsf{R})$ are two monotone set multifunctions such that $\mu_1(\varnothing) = \mu_2(\varnothing) = \{0\}$ and $\mu_1(A) \subseteq \mu_2(A)$, for every $A \in \mathsf{C}$ (for instance, one can think to $\mu_1, \mu_2 : \mathsf{C} \to \mathsf{P}_f(\mathsf{R})$, $\mu_1(A) = [0, m_1(A)], \mu_2(A) = [0, m_2(A)]$ for every $A \in \mathsf{C}, m_1, m_2 : \mathsf{C} \to \mathsf{R}_+$ being monotone, $m_1(A) \leq m_2(A)$, for every $A \in \mathsf{C}$, $m_1(\varnothing) = m_2(\varnothing) = 0)$. Then any minimal atom of μ_2 is a minimal atom of μ_1.

(ii) Let be $\mu : \mathsf{C} \to \mathsf{P}_f(\mathsf{R}), \mu(A) = [-m_1(A), m_2(A)]$ for every $A \in \mathsf{C}$, where $m_1, m_2 : \mathsf{C} \to \mathsf{R}_+$, $m_1(\varnothing) = m_2(\varnothing) = 0$. Then a set $A \in \mathsf{C}$ is a minimal atom of μ iff A is a minimal atom for both m_1 and m_2 in the sense of (Mesiar *et al*., 2017; Ouyang *et al*., 2015).

(iii) If $\mu : \mathsf{C} \to \mathsf{P}_f(\mathsf{R}), \mu(A) = \{m(A)\}$, for every $A \in \mathsf{C}$, where $m : \mathsf{C} \to \mathsf{R}_+$, $m(\varnothing) = 0$, then a set $A \in \mathsf{C}$ is a minimal atom of μ iff A is a minimal atom for m in the sense of (Mesiar *et al*., 2017; Ouyang *et al*., 2015).

In this way, one sees that Definition 3.1 - (i) generalizes to the set valued case the corresponding notion introduced by (Mesiar *et al*., 2017; Ouyang *et al*., 2015).

Definition 3.7 (i) *If* $\mu : \mathsf{C} \to \mathsf{P}_f(X)$, *let be the variation of* μ, $\overline{\mu} : \mathsf{P}(T) \to [0, \infty]$, *which is defined for every* $A \in \mathsf{P}(T)$ *by:*

$$\overline{\mu}(A) = \sup\left\{\sum_{i=1}^{p} |\mu(A_i)|; A = \bigcup_{i=1}^{p} A_i, A_i \in \mathrm{X}, \forall i = \overline{1, p}, A_i \cap A_j = \varnothing, i \neq j\right\}.$$

(ii) *We say that* μ *is of finite variation if* $\overline{\mu}(T) < \infty$.

Remark 3.8 For every $A \in \mathcal{C}$, we have $\overline{\mu}(A) \geq |\mu(A)|$. Consequently, if $A \in \mathcal{C}$ is a minimal atom of $\overline{\mu}$ in the sense of (Mesiar *et al*., 2017; Ouyang *et al*., 2015), then A is a minimal atom of μ.

Conversely, if $A \in \mathcal{C}$ is a minimal atom of μ, then it is also an atom of μ, so $\overline{\mu}(A) \geq |\mu(A)|$, whence A is a minimal atom of $\overline{\mu}$.

Remark 3.9 (i) Any set $A \in \mathcal{C}$ that can be written as $\bigcup_{i=1}^{p} A_i$ (where for every $i = \overline{1,p}$, $A_i \in \mathcal{C}$ are different minimal atoms of μ), is partitioned in this way, since by Proposition 3.3 we have $A_i \cap A_j = \emptyset$, $i \neq j$.

Since any minimal atom is an atom, then in this case $\overline{\mu}(A_i) = |\mu(A_i)|$, for every $i = \overline{1,p}$. Consequently, if, moreover, μ is a multisubmeasure of finite variation in the sense of (Gavriluţ, 2009), then by (Gavriluţ, 2009), $\overline{\mu}$ is finitely additive, so $\overline{\mu}(A) = \sum_{i=1}^{p} |\mu(A_i)|$.

(ii) (non-decomposability of minimal atoms) Any minimal atom $A \in \mathcal{C}$ can not be partitioned (its only partition is $\{A, \emptyset\}$).

The converse of the last statement also holds:

Proposition 3.10 *Any non-partitionable atom* $A \in \mathcal{C}$ *is a minimal atom.*

Proof. Since A is an atom, then $\mu(A) \supseteq \{0\}, \mu(A) \neq \{0\}$. On the other hand, because A is non-partitionable, there can not exist two nonvoid disjoint subsets of A, let us say $A_1, A_2 \in \mathcal{C}$.

Let be now arbitrary $B \in \mathcal{C}$, with $B \subseteq A$. One has either $\mu(B) = \{0\}$ or $\mu(B) \supseteq \{0\}, \mu(B) \neq \{0\}$. In the latter situation, we can have only $B = A$ (if not, $\{A \setminus B, B\}$ is a partition of A, which is a contradiction).

Corollary 3.11 *An atom is minimal if and only if it is not partitionable.*

Theorem 3.12 *If* T *is finite,* μ *is null-additive and* $\{A_i\}_{i=\overline{1,p}}$ *is the set of all minimal different atoms contained in a set* $A \in \mathcal{C}$, *with* $\mu(A) \supseteq \{0\}, \mu(A) \neq \{0\}$, *then* $\mu(A) = \mu(\bigcup_{i=1}^{p} A_i)$ *(so, the minimal atoms are the only ones which are important from the "measurement" point of view).*

Proof. $\mu(A \setminus \bigcup_{i=1}^{p} A_i) = \{0\}$ (if not, there exists another minimal atom of μ). By the null-additivity of μ, one gets $\mu(A) = \mu(\bigcup_{i=1}^{p} A_i)$.

4. From the Standard Mathematical Atom to the Fractal Atom by Means of a Physical Procedure

Let T be an abstract nonvoid set, C a lattice of subsets of T and $m: \mathsf{C} \to \mathsf{R}_+$ an arbitrary set function with $m(\varnothing) = 0$. One can immediately generalize the notions of a pseudo-atom / minimal atom, respectively, to the case when C is only a lattice and not necessarily a ring.

Example 4.1 (i) It T is a nonempty metric space, then the Hausdorff dimension $\dim_{Haus}: \mathsf{P}(T) \to \mathsf{R}$ (Mandelbrot, 1983) is a monotone real function. Evidently, $\dim_{Haus}(\varnothing) = 0$.

(ii) For every $d \geq 0$, the Hausdorff measure $H^d : \mathsf{P}(T) \to \mathsf{R}$ is an outer measure, so, particularly, it is a submeasure.

Remark 4.2 (i) The union of two sets A and B having the fractal dimensions D_A, respectively, D_B has the fractal dimension $D_{A\cup B} = \max\{D_A, D_B\}$;

(ii) The intersection of two sets A and B having the fractal dimensions D_A, respectively, D_B has the fractal dimension $D_{A\cap B} = D_A + D_B - d$, where d is the embedding Euclidean dimension (Iannaccone and Khokha, 1995).

The following definition is then consistent:

Definition 4.3 *A pseudo-atom / minimal atom, respectively, $A \in \mathsf{C}$ of m having the fractal dimension D_A is said to be a fractal pseudo-atom / fractal minimal atom, respectively*.

One can easily verify the following:

Proposition 4.4 *If $A, B \in \mathsf{C}$ are fractal pseudo-atoms of m and if $m(A\cap B) > 0$, then $A\cap B$ is a fractal pseudo-atom of m and $m(A\cap B) = m(A) = m(B)$.*

5. Concluding Remarks

The main conclusions of the present paper are the following:

i) Minimal atomicity in correspondence with Quantum Measure Theory is discussed and some physical applications are provided;

ii) The concept of atomicity (and, particularly, of minimal atomicity) is extended in the form of fractal atomicity, respectively, fractal minimal atomicity. Some mathematical properties of fractal minimal atomicity are given.

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VARIANTE ALE ATOMICITĂŢII ŞI UNELE APLICAŢII FIZICE

(Rezumat)

În această lucrare, prezentăm unele rezultate referitoare la diferite forme de atomicitate din perspectiva teoriei măsurii cuantice şi stabilim câteva aplicaţii în fizică. Mai precis, extindem conceptul matematic de atomicitate minimală şi, pe baza remarcii conform căreia mecanica cuantică este un caz particular de mecanică fractală la o rezoluţie de scală specifică, introducem conceptul de atomicitate fractală (şi, în particular, cel de atomicitate minimală fractală). De asemenea, indicăm unele proprietăţi matematice ale acestora.

BULETINUL INSTITUTULUI POLITEHNIC DIN IAŞI
Publicat de
Universitatea Tehnică „Gheorghe Asachi” din Iaşi
Volumul 64 (68), Numărul 2, 2018
Secţia
MATEMATICĂ. MECANICĂ TEORETICĂ. FIZICĂ

SAGITTARIUS A*: A COMPELLING CASE AGAINST THE EXISTENCE OF A SUPERMASSIVE BLACK HOLE IN THE CENTER OF MILKY WAY

BY

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Received: April 10, 2018
Accepted for publication: May 18, 2018

Abstract. The astrophysics literature tries to make a case for the existence of a supermassive black hole at the center of Milky Way, in the location of the radio source Sagittarius A*. We think that, with arguments of the very same nature, the evidence points quite to the contrary. Thus, while the observational data on the orbits of the starry objects around Sagittarius A*, being of a projective character, are entirely reliable, their physical explanation uses quite a particular type of Newtonian forces, namely those with magnitude depending exclusively on the distance between bodies. To begin with, this limitation assumes a priori that the bodies connected by such forces are special material points, viz. space positions endowed with mass. At space scales such as that of the galactic center region in discussion, this assumption is not realistic, and therefore, implicitly, such particular forces are themselves not quite realistic. Still using Newtonian forces in argument, one should allow, on such an occasion, their full generality. This means that we only need to assume that they are central forces with no other further constraints. Within the framework of the Newtonian theory of forces this freedom has important theoretical consequences discussed in the present work. Among these the chief one, from astrophysical point of

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view, is that the presence of a supermassive black hole in the center of Milky Way might not be a sustainable assumption. An alternative is presented.

Keywords: Sagittarius A*; Milky Way; central forces; Newtonian theory of forces; electromagnetic field; production of field; astrophysics; fundamental physics.

1. Introduction

We note that a previous version of this work was uploaded to the online free access database *viXra.org* (Mazilu, 2012).

The story starts with the discovery of the galactic radiosource called Sagittarius A* in the center of the Milky Way (Balick and Brown, 1974). The scientific consensus is that, physically, such a source should be correlated with the existence of a material body in that place. For, the fundamental physical notion is that the electromagnetic field is only created by the motion of matter. However, such a body is optically invisible at that position. And as, according to fundamental physical understanding, one cannot presume that the center of a spiral galaxy is simply an empty location emitting electromagnetic radiation, the astronomers got quite a mystery in their hands.

Then, later on, the adaptative optics stepped down from the military to scientific uses, and starting from about the beginning of the last decade of the previous century, it allowed to astrophysicists distinguishing starry isolated objects moving against the background of the center of the Milky Way. It was thus possible to notice coherent patterns in the motion paths of such stars, as projected on the canopy (for an outstanding review of the history, evidence and elimination of the many alternative physical explanations see (Reid, 2009) and the original literature cited there). One such object, called S02, even completed an elliptic path, under our eyes so to speak, in about 16 years, proving beyond any doubt that its motion is Keplerian. Further analysis revealed many such gravitating stars, whose paths are only partially accessible though. Nevertheless their observed positions are enough for allowing astrophysicists to infer that their complete orbits are ellipses.

The common feature of all these orbits is that they all contain the radiosource Sagittarius A* in one of their foci, therefore they should be Keplerian orbits, or at least very close to these. And as this source is dim in any kind of perturbations that can reach the Earth, one can easily suspect that not all radiation comes out from the source. First, the object is invisible. Therefore the optical part of the spectrum does not reach the Earth, and this can have a rational explanation: it is swallowed by the matter existing between the center of the Milky Way and the solar system. This seems only reasonable, inasmuch as the matter between the center of galaxy and the solar system dims the light by some 30 orders of magnitude. In other regions of spectrum we are luckier: infrared and radio waves are dimmed only by about three orders of magnitude.

However, there is still a big discrepancy between the mass to be assigned to the body assumed to create the gravitational field responsible for the motions of those stars and the amount of radiation we are supposed to receive from such a body. This fact helped gradually built the conclusion that the central body works in the way in which a black hole is supposed to work. For, if one applies the Newtonian theory of forces in a classical way (see for instance (Gillessen, 2009)), the mass of an object that fits the requirement of being the source of such a gravitational field is about four million and a half solar masses: a supermassive black hole!

Recently, a new finding, seems to support the idea of a massive black hole in the center of Milky Way:

"Recently, we discovered a peculiar molecular cloud, CO–0.40–0.22, with an extremely broad velocity width, near the centre of our Milky Way galaxy. Based on the careful analysis of gas kinematics, we concluded that a compact object with a mass of about $10^5 M_\odot$ is lurking in this cloud. Here we report the detection of a point-like continuum source as well as a compact gas clump near the centre of CO–0.40–0.22. This point-like continuum source (CO–0.40–0.22*) has a wide-band spectrum consistent with 1/500 of the Galactic SMBH (Sgr A*) in luminosity. Numerical simulations around a point-like massive object reproduce the kinematics of dense molecular gas well, which suggests that CO–0.40–0.22* is one of the most promising candidates for an intermediate-mass black hole" (Oka *et al*., 2017).

As seen in the paragraph above, this new data was interpreted using numerical simulations based on the same classical assumptions as the ones before it (Reid, 2009).

It is our opinion that the very theory of forces used to disentangle such a case is not completely adequate to the task, so the conclusion of the existence of a black hole in the center of Milky Way, or in the center of any other galaxy for that matter, might not be the appropriate one. In fact the observational data may be pointing out to the necessity of approaching the physics of the center of Milky Way with the ingenuity with which Newton himself approached its prototype, the Keplerian synthesis of planets' motion. Thus, while we agree entirely with the statement that the Milky Way's center is "a laboratory for fundamental astrophysics and galactic nuclei" (Ghez *et al*., 2005), we think a little further, namely of 'a laboratory for *fundamental physics*' at large. For, the data itself may compel us to change the ideas about the fundamental forces as we claim to know them today, by looking deeper into their history and considering it face value.

Indeed, we are, here and now, in that unique situation in which the science was only once in its history. That was in the times when Newton, having at his disposal the Keplerian synthesis of Tycho Brahe's data on Mars, has invented the forces of which the physicists and astronomers speak today. Thus, on one hand, we have at our disposal the outstanding synthesis, allowed

by the adaptative optics, of the motions of the stars in the very central part of our galaxy (see (Ghez *et al*., 2005; Eckart *et al*., 2002) and the earlier original works cited there). Like the old Kepler synthesis, the new synthesis points out to coherent motions, of stars this time, which projected on the canopy appear as elliptical motions. Therefore, in reality they cannot be but Keplerian motions, no matter of the orientation of their planes in space. Being based on projections on the canopy, the conclusion is by no means affected by the uncertainty in the galactic metric parameters (for a recent critical study of such uncertainties see for instance (McMillan and Binney, 2010)). It is therefore the most reliable conclusion one can draw based on observations. Now, when the orientation of those planes of motion is taken into consideration in extracting the orbits from the data, all these orbits reveal that Sagittarius A* is in one of their foci, just like the Sun in the Kepler's case. But unlike the planets of the solar system, the stars orbiting around Sagittarius A* are not in the same plane. All we can say is that as conic sections they belong to a family of quadrics having a common focus. This fact may, by itself, indicate that the case of the black hole is unsustainable.

For, on the other hand, the usual physical explanation of this observational synthesis stops at some quite particular class of forces that might not be appropriate to the task. These forces are assumed to be well known, being of the type which Newton used in order to explain the ideal Kepler motions, amended, on occasions, to account for the almost insignificant rotations of the orbits. In fact, with rare exceptions, the whole speculative physics today uses only such forces, distinguished by the fact that they are conservative and have the magnitude depending exclusively on the distance between the attracted and the attracting bodies. Provided, of course, these bodies can be considered material points in the classical sense, *i.e.* space positions endowed with physical properties (mass, charge etc.).

So, regarding the main physical argument used in explaining the observational data – the forces – we think that it calls for a more careful consideration. Specifically, we should go way deeper with the assumptions about the forces responsible for the contemporary Kepler motions in the center of Milky Way, at least as deep as Newton went in the prototypical case of the original Kepler motion. It appears therefore as only appropriate to start our present undertaking with the essentials of Newton's approach of his invention of central forces (see (Newton, 1995) Book I, Sections II & III).

2. The Newtonian Forces

In order to make our message more clear, let us rephrase the Corollary 3 of the Proposition VII from *Principia*, with reference to an arbitrary orbit, not just a Keplerian one. This confers maximum generality to the concept of Newtonian force and to its quantitative definition, pointing out the particular

situation of the mass itself in the construction of force. This corollary is, in our opinion, the key of understanding the action of all forces in the universe. In a simplified expression, extracted from Newton's original (Newton, 1995, p. 48), and adapted for our specific needs, it sounds like:

The force by which a body P … revolves about a center of force S, is to the force by which the same body may revolve *in the same orbit, and the same periodic time, about another center of force* R, as the volume SP×RP2, … to the cube of the straight segment SG, drawn from the first center of force S, parallel to the distance RP of the body from the second center of force R, and meeting the tangent PG of the orbit in G. One can easily draw a figure in order to better assess the geometrical situation. The points S and R can occupy *any positions* with respect to the observed orbit in its plane.

To our knowledge, J.W.L. Glaisher appears to be the first one who properly put this statement into an analytical form, with no recourse whatsoever to dynamical principles, and with reference to the eliptic, therefore closer to Keplerian, form of the orbit (Glaisher, 1878). The theory goes, by and large, along the following lines. Assume that, in the Cartesian coordinates of the plane of motion, the equation of the observed orbit is the quadratic non-homogeneous equation

$$f(x,y) \equiv a_{11}x^2 + 2a_{12}xy + a_{22}y^2 + 2a_{13}x + 2a_{23}y + a_{33} = 0 \qquad (1)$$

Then the relation between the two forces expressed in the statement above can be translated into equation:

$$\text{FORCE toward } S = (1+\vec{\xi}\cdot\vec{\varepsilon})^3 \frac{r}{\sqrt{r^2+\varepsilon^2-2\vec{r}\cdot\vec{\varepsilon}}} \cdot (\text{FORCE toward } R) \qquad (2)$$

Here $\vec{\xi}$ the vector of components

$$\frac{a_{11}x + a_{12}y + a_{13}}{a_{13}x + a_{23}y + a_{33}}, \quad \frac{a_{12}x + a_{22}y + a_{23}}{a_{13}x + a_{23}y + a_{33}} \qquad (3)$$

and $\vec{\xi} \equiv \overrightarrow{SR}$. $\vec{r}$ denotes here the position vector of the moving point *P* with respect to *S*, and *r* is its magnitude – *i.e.* what we call here the distance, when not otherwise specified.

Eq. (2) shows how to calculate analytically the force in *P* toward point *S*, when we happen to know the force in *P* toward the point *R* from the plane of motion. This is the basic mathematical principle of the Newtonian natural philosophy. It is not hard to see that it extends… naturally the observations related to the 'working principle' of a sling shooting, whereby the force of gravity – *i.e.* the weight – acting vertically, is actually 'compared', by means of the sling itself, with the centrifugal force, acting horizontally or in any other direction.

Now, the force toward *R* can be taken as reference in measuring the force in the current point *P* of the orbit *in any other direction*. So, in this case, we are sort of compelled, so to speak, to a choice of *R* that makes the theory of forces universal, at least in the Keplerian situations. This leads within modern theoretical physical views, to a calibration of Newtonian forces. In the cases where *R* occupies the position of *the center of the orbit*, Newton has inductively shown that the force toward it, is directly proportional with the distance between *R* and *P*, *i.e.* with the distance from the center to the orbiting point. If we use this result in Eq. (2), then the force we need to know is

$$\text{FORCE toward } S = \mu \cdot r \cdot (1 + \vec{\xi} \cdot \vec{\varepsilon})^3 \tag{4}$$

where μ is a constant of proportionality, coming from the force toward the center of orbit. If, further on, we use the components (3) of the vector $\vec{\xi}$, we get:

$$\text{FORCE toward } S = \mu \cdot a_{33}^2 \cdot \frac{r}{(a_{13}x + a_{23}y + a_{33})^3} \tag{5}$$

in the reference frame where *S* is in origin. This result can be, of course, expressed in different manners, depending on the way of writing the equation of the conic representing the orbit. However, it carries an even more important message, at least from a geometrical point of view.

With the substantial help of the analytical geometry of conics, in words the result sounds: *the force toward a certain center by means of which a certain material point describes a conical orbit around that center, is directly proportional to the distance from the point to the center of force and inversely proportional with the third power of the distance from the point to the straight line conjugated to the center of force with respect to the orbit*. This is a theorem first given by W.R. Hamilton (Hamilton, 1847) on the "occasion of a study of *Principia*." Therefore, once again, the center of force can occupy any position with respect to the orbit, but in the case of conical orbits, and with a standard choice of the reference force, *i.e.* in a standard calibration or gauging of the forces, the definition of Newtonian force involves the very same elements as the definition of the orbit itself: the distances of the generic point of orbit from the center of force and from the polar line coresponding to that center of force.

This fact should be more obvious if we write the equation of force in the form:

$$f(x, y) = \frac{\mu r}{[(a_1x + b_1y + c_1)(a_2x + b_2y + c_2)]^{3/2}} \tag{6}$$

Here the equation of the orbit is understood in the form

$$(a_1x+b_1y+c_1)(a_2x+b_2y+c_2)-(a_{13}x+a_{23}y+a_{33})^2=0 \qquad (7)$$

It expresses the fact that, geometrically, the orbit is determined by its tangent lines – real or imaginary – in the two points where the straight line polar to the center of force with respect to the orbit cuts it. The tangents are considered as having the equations:

$$a_1x+b_1y+c_1=0; \quad a_2x+b_2y+c_2=0 \qquad (8)$$

while the polar itself of the center of force with respect to the orbit is taken as given by equation

$$a_{13}x+a_{23}y+a_{33}=0 \qquad (9)$$

Now, based on this general presentation, let's see where the limitation to the dependence of the magnitude of force exclusively on the distance enters the physics of gravitating systems. For, one can see from Eq. (6) that, in general, such a behavior of the magnitude of force is far from being the general case. Rather, the magnitude of the Newtonian force as we read it even in conical orbits, with no further specification of the position of the actual center of force, *depends also on the current direction of the orbiting body*.

The very idea of force in explaining celestial harmony started from the first of the Kepler laws: the planets describe elliptical orbits *with the Sun in one of their foci*. This last information is crucial. For, if the position of the center of force is in a focus of the ellipse, then the magnitude of force *cannot depend but on the distance*, and that even in a very special way. Indeed, we can then use the equation of the orbit referred explicitly to one of its foci. By the definition of a conic section, the ratio between the distances from the planet to one of the foci and from the planet to the corresponding directrix (the polar of focus) is constant: the eccentricity. This comes down analytically to the equation

$$r^2=e^2\cdot(a_{13}x+a_{23}y+a_{33})^2 \qquad (10)$$

where e is a number proportional to the eccentricity of the orbit. In this case, using the Eq. (7), Eq. (6) leads directly to:

$$f(x,y)=\frac{\mu}{r^2} \qquad (11)$$

with μ – a constant. This is the force of 'universal gravitation' to which the classical physics makes always reference, with no mention though of the prerequisites of its expression: that the point of attraction and the point attracted

have to be only… points, and furthermore, the point of attraction has to occupy a privileged position with respect to orbit – that of one of its foci. For, if the point of attraction occupies any other position in the plane of motion, with rare exceptions, we may be in the situation that the magnitude of force depends also on the direction from the center of force to the moving body. Thus the universally used Newtonian force of gravity is actually quite a particular choice among the possible forces responsible for the Kepler synthesis.

Let's therefore see what other cases may occur of dependence of the magnitude of Newtonian forces only on distance. Indeed, the motion of planets is not the only one given to our experience, although we have to recognize that it is the one that stirred up everything. Thus, for instance, the immediate experience has certainly to do with with elastic forces too. These are the forces that 'gauge' – and that in a quite precise manner we should say (see (Mazilu and Agop, 2012)) – all the modern positive science, insofar as it needs to be submitted to experimental verification. And such forces are obtained, within the Newtonian program sketched above, in cases where the center of force coincides with the center of the orbit. In Eq. (7) this means $a_{13} = a_{23} = 0$, and therefore Eq. (6) becomes:

$$f(x, y) = \mu \cdot r \tag{12}$$

where μ is another constant, not necessarily that from Eq. (11). This might seem as a tautology – we started specifically from the idea that the force toward the center of the orbit is an elastic one – but, at a closer scrutiny we might have to change this opinion. First of all, Eq. (12) shows that the theory is not self-contradicting, and this is an important fact by itself. Secondly, this shows that the Newtonian formula works for the same point in the plane of orbit *in two different instances* – as material point and empty position – and this is most important conclusion for theoretical physics.

3. The Concept of Field and the Modern Idea of Gauging

Indeed, this is the very essence of the *idea of field* in physics. For a better understanding, consider the situation of light. What we usually accept is that the Newtonian force is proportional to distance in the cases where the center of force is material and located in the center of the orbit. What about the cases when *that center of force is simply an empty position*? This is plainly the case of the Fresnel ellipse in the plane waves of light, perpendicular to the light ray: there is no material center of force on the light ray, and yet the light can be described as if there is one there. This fact reveals the real merit of the Newton's definition of the force: it can be calculated with respect to any point, once the geometric setup is Keplerian! The force has indeed the characteristics

of a true field, as these came down to us from the theoretical physics of the 19th century. This would mean, for instance, that in the case of a light ray there is always a Newtonian central force *acting along the ray*, toward or away from the source of light. The idea was always rejected from the realm of physics, based exclusively on the fact that the force should be a vector, for which the formulas like (11) and (12) give the magnitude unconditionally. As Glaisher's analysis clearly shows, this was not at all the case when Newton has invented the forces.

Regarding the light phenomenon per se, this philosophy was materialized even from the times of Fresnel, by the 'gauging' proposal of James Mac Cullagh (Mac Cullagh, 1831) for the *representation of the light according to Newtonian view of forces*. Let us briefly see what Mac Cullagh's point of view is about. He was concerned with the elliptically polarized light, like the light passing through rock crystals. He found that this light can be represented by two harmonic vector processes in the same plane, like the processes invented by Fresnel to help explaining the light phenomenon, making a certain angle between them. Later on (Mac Cullagh, 1836) he noticed that the theory can be put in a space-time form by a system of coupled differential equations, which led him to the foundations of a theory of ether (Mac Cullagh, 1839) – improved afterwards by Lord Kelvin and Joseph Larmor – and finally to an exquisite explanation of the phenomenon of double refraction in quartz (Mac Cullagh, 1840). It is to be noticed that the veiled persuading argument of Mac Cullagh's feat seems to have been the faulty notion of describing the light by a displacement, advanced initially by Fresnel. Indeed, in the case of light – a continuum phenomenon – the mechanical displacement has no object, *i.e*. it is not referring to a material point, but simply to an empty position in space, for no matter as we know it is located there. This very fact made Newton's natural philosophy hardly relevant to the light, a detail corrected, as we see, in a brilliant way by Mac Cullagh. These observations explain, by and large, the almost explicit contribution of Mac Cullagh to the future electromagnetic theory of light (Darrigol, 2002; Darrigol, 2010). In hindsight though, Mac Cullagh's seems to us to be much more than an electromagnetic theory. It should be taken, indeed, as the very first specimen of a gauge theory (see 10 for a discussion of light in 'Mac Cullagh's gauge') of the kind that came into existence more than a century afterwards, in the form of the Yang-Mills theory (Yang and Mills, 1954).

Returning, for one last consideration, back to the Eqs. (11) and (12), they reveal forces whose magnitude is exclusively dependent only on the distance between the points assumed to be physically correlated by them. These happen also to be the only forces that satisfy the Kepler geometry per se, *i.e*. the only ones having *closed orbits* (Bertrand, 1873). But one can see from these examples that the dependence of the magnitude of force exclusively on distance is acquired, first of all, by the *special position of the center of force* with respect to the orbit. Secondly, and by no means less important, is the fact that the universal 'comparison force' as it were, the gauging force of the Newtonian

procedure, is the elastic force, which may or may not be actual after all, when referred to criteria dictated by our senses, depending on the circumstance that the center of orbit contains matter or not. And any other comparison force than the elastic isotropic one, used in the Newtonian procedure of defining forces, would make the formula (6) more complicated, perhaps even prohibitively. This moment in the definition of force in the Newtonian philosophy turns out to have universal significance even through the modern idea of 'gauging' from theoretical physics. From this perspective it shows even more: nothing can be reproducibly described in physics, unless we have a gauge for it.

Nevertheless, it turns out that the Eqs. (11) and (12) are used nowadays in theoretical physics with no reference to their Newtonian foundation, and therefore with no further qualifications about their very possibility at that. For instance there are times, and very often at that, when the force from Eq. (11) is considered a static force. This should entail special considerations, because originally the very existence of such force carries a precise identity: it is clearly related to a Keplerian motion, and moreover, the value (11) is referred to a gauging elastic isotropic force that might not even be actual. In hindsight though, judging by the success of such universal 'anonymous' forces in the history of physics, specifically in the theory of light and astrophysics, there seem to be no need at all for the existence of matter in the center of the conic, in order to ratify their reality. If one needs a ratification anyway, this comes simply from the fact that the elastic forces are an expression of the existence of a privileged coordinate system – that of *harmonic coordinates* (Mazilu and Agop, 2012).

In the case of those two time-honored central forces with magnitude depending exclusively on distance, we have as centers of force the very center of the orbit and its focus. But these are by no means singular cases leading to a force with magnitude depending exclusively on distance. If, for instance, the motion is elliptic and the center of force is located on the orbit itself, the magnitude of the force accounting for this motion is inversely proportional with the fifth power of the distance. By the same token, if the orbit is of a special shape – other than a conic section – we may also have forces exclusively depending on distance. This is, for example, the case when the motion has the space form of a logarithmic spiral, like the arms of a galaxy. The force accounting for such a motion pulls toward the pole of the spiral with a magnitude inversely proportional with the third power of the distance from that center.

The case presented by Sagittarius A* is outstanding mostly from a special point of view of natural philosophy, that may induce us to reconsider the previous old natural philosophy founded by Newton. As we have already mentioned above, *the only criterion that validates the decision that a body is acted upon by a force pulling towards a certain point in space is the perceived matter in that point*. This can be actually quoted as the first gauging criterion of physics. It turns out to work even today in full swing. According to this

criterion, Sagittarius A* should be such a point, even though only 'partially perceived' as it were. However, it does not satisfy itself to another criterion that historically became essential, but actually it turned out to be quite arbitrary: *that of mass*. In order to define this criterion, and to recognize its true meaning, let's follow the evolution of Newtonian ideas along the theory of continuum material, leading to Poisson's equation. This is actually the route which led to the modern theoretical physics' idea of gauging in the first place.

4. The Mass and the Newtonian Theory of Forces

Perhaps we would have never talked about the whole theoretical physics as it is today, if Newton would not have insisted on the idea that the force of gravity should be directly proportional with the 'quantities of matter' of the bodies involved in the interaction represented by that force. More precisely, in modern vector notation, the Newtonian force created by a body of mass M on a body of mass m, can be written as

$$\vec{f}(\vec{r}) = -G\frac{Mm}{r^2}\frac{\vec{r}}{r} \tag{13}$$

Here G is the so-called gravitational constant, and $\vec{r}$ is the position vector of m with respect to *M*, again, both *considered as material points*. Now this force can be thought of as existing by itself, separated from its roots as it were, *i.e.* disregarding its Keplerian origin. As we have mentioned before, it can even be considered a static force. The physical problem now moves on to the realm of mechanics: can this force explain the observed motions? and how? The answer is well known, and resides in the principles of dynamics, put forward by Newton in order to be able to profitably use the force. This time though, the force is assumed to be the independent cause of the motion.

Our way of writing the force here points to the fact that the force is attractive, being opposite to the orientation of the position vector. Its magnitude does not depend but on the distance between the two material points assumed to be correlated by force, and this in a very special way, shown above in Eq. (11) as specific to a Keplerian setting involving an elliptical orbit with the center of force in one of its foci:

$$f(\vec{r}) = G\frac{Mm}{r^2} \tag{14}$$

Therefore $\mu \equiv GM$ in formula (11) above.

Newton insisted at length on the fact that the force of gravitation should be proportional with the quantities of matter of both bodies involved in the interaction represented by force, otherwise nothing would make sense. This is a

rather arbitrary assumption by itself (for *the only* critical approach of the issue, at least as far as we can judge, see (Poincaré, 1897; Poincaré, 1921)). It was like Newton was mindful of the fact that, some two hundred years after him, the general relativity would have to come into existence, and he ought to create its possibility. However, he was apparently guided in his insistence only by the fact that a force like that from Eq. (14) is able to offer physical support to the marvelous synthesis by Kepler of the motion of the planet Mars.

Indeed, in modern terms, in order to obtain the Kepler laws it is sufficient to solve the Newtonian equations of motion written in the form

$$\ddot{\vec{r}} + \frac{K}{r^2}\frac{\vec{r}}{r} = \vec{0} \tag{15}$$

as one proceeds routinely today. Here $K \equiv GM$, and so it is obvious that the description of motion by this equation is universal even in the more precise sense that it does not depend on the mass of the moving body. So, if the independence of the force (13) of its physical origin could still be counted as an arbitrary assumption, the undeniable success of the mathematics handling of Eq. (15) bestows upon it an equally incontestable actuality. For, this is the first moment where the idea of field, independent of matter, came up to science.

The Newtonian force from Eq. (13) is conservative, *i.e.* can be derived from a potential. The existence of a potential in the problem of classical gravitational field means however more than the mere law of conservation of the mechanical energy. It also opens the path of speculations regarding the structure of matter and of the characterization of a continuum from mechanical point of view, as initiated by Newton himself. In order to show this, let us notice that we can write the Newtonian force in the form

$$\vec{f}(\vec{r}) = m\nabla V_1(\vec{r}); \quad V_1(\vec{r}) \equiv \frac{GM}{r} \tag{16}$$

where ∇ is the operation of gradient and V_1 is the potential energy. Considering only the force per unit mass, the force from Eq. (16) is:

$$\vec{f}(\vec{r}) = \nabla V_1(\vec{r}) \tag{17}$$

This force is therefore an intensity, characteristic of the space around the mass assumed to exert that force. It is this space, thus physically characterized, that came to be known as a field: *the gravitational field*. The force exists in every point of space, no matter of the other physical properties of that point: it can be simply a position in space, as well as the location of a

material particle. Therefore the force is a continuous vector function of the position in space, and can very well be a characteristic of a material continuum filling the space. Which characteristic was not so long in coming to physical considerations, being, as it were, a necessity forced upon the mathematics of natural philosophy by the space expansion of material bodies.

Indeed, inasmuch as one can think of a physical structure of a material continuum, this gives us the right to calculate the flux of force around a certain point in space. Considering the force from Eq. (13) as a static force, we can use a spherical surface around origin of coordinates. If we calculate its flux through a spherical surface of radius *r* according to the usual formula

$$\oiint_{Sphere} \hat{n} \cdot \vec{f}(\vec{r}) dA \tag{18}$$

where $\hat{n}$ is the unit normal to the sphere and dA is its elementary area, we get an interesting result. As the unit normal vector to the sphere is just the versor of the position vector, and $dA = r^2 \sin\theta d\theta d\varphi$, we have

$$\oiint_{Sphere} \hat{n} \cdot \vec{f}(\vec{r}) dA = 4\pi GM \tag{19}$$

Therefore the flux of force of the gravitational field is, up to a universal factor, the mass of the material point creating the field – appropriately called the source of field. Now, the mass of that source can be represented, according to Newton's definition of the density of matter (Newton, 1995, p. 9), by a volume integral:

$$M = \iiint_{Volume} \rho(\vec{r}) d^3\vec{r} \tag{20}$$

where $\rho()$ denotes the Newtonian density at the chosen location and $d^3\vec{r}$ is the volume element at the same location. Using the Eqs. (17), (19) and (20) we get

$$\oiint_{Sphere} \hat{n} \cdot \nabla V_1(\vec{r}) dA = 4\pi G \iiint_{Volume} \rho(\vec{r}) d^3\vec{r} \tag{21}$$

where the 'Volume' is that of the corresponding 'Sphere'. Further on, using Gauss' theorem for the left hand side of this equation, we have

$$\iiint_{Volume} \left\{ \nabla^2 V_1(\vec{r}) + 4\pi G\rho(\vec{r}) \right\} d^3\vec{r} = 0 \tag{22}$$

In fairly general continuity conditions, the integrand of this equation should then be zero. This gives us the Poisson's equation, relating the Newtonian density of matter that generates the field to the field potential. Usually, the potential is taken without the gravitational constant, which comes to a simple redefinition: $V_1 = GV$. So, the equation of Poisson becomes the one we usually write today:

$$\nabla^2 V(\vec{r}) = -4\pi\rho(\vec{r}) \tag{23}$$

This is the equation which, from the perspective of general relativity for instance, is the fundamental equation of the classical mechanics. It is not usually considered quite by itself, but in conjunction with the implicit idea that *we are always able to know the density of matter*. It is therefore an equation giving us forces, when knowing that we have at our disposal the matter creating, as it were, these forces, provided that one can characterize this matter by a density in the Newtonian recognition. More than this, it contains, in the background at least, the idea that the material point of Newton is not simply a position in space, as actually the rigorous calculation requires: it should be endowed with a space expanse to be occasionally considered. It is in this general acceptance that the equation is used in characterizing the Sagittarius A* case.

Now, obviously, by Eq. (20), and therefore by Eq. (23), we actually describe the part of space *inside the matter*. Then, the Poisson's equation itself becomes part of fundamental physics. Indeed, it is really necessary in the description of nature, inasmuch as it provides us knowledge on the space inside matter. The hard part of the problem is that the Newtonian density is only a hypothesis, and quite unreliable at that, because the matter is not inherently homogeneous with respect to space, and we do not have access to its space details – at least not always. Nevertheless, within certain quite natural assumptions, that knowledge is inferrable, as it was actually the case all along the time. The most reliable, and the only one entirely realistic we should say, of these assumptions is offered by the particular case of the Poisson's equation, where the density of matter is zero, viz. *the Laplace equation*. Indeed, the Newtonian potential of the force from Eq. (13) above is actually a solution of Laplace equation, thus characterizing the situation in vacuum. And this fact is quite natural: the Newtonian force has not been invented otherwise, but specifically for describing the interaction between *material points in vacuum*. It is only its extension to the space inside matter – allowed by the equation of Poisson, *which in turn was allowed by the special assumption of Newton on the position of masses in the expression of the magnitude of force* – that creates the impression that the force depends physically on the density of matter. This line of thought was initiated indeed by Poisson in 1812, and put on mathematical firm grounds by Gauss in 1839 (see (Gauss, 1842)). It is along it, that Einstein

found flaws to classical physics, and thus pressed forward the ideas that led to the general relativity. A brief history of the main points of development of the theory is perhaps in order.

In 1812 Poisson noticed that inside matter the law of attraction between different material points cannot be the law of Newton, because the potential cannot satisfy there a Laplace equation (Poisson, 1812). He has actually noticed that the Newtonian density of matter becomes instrumental there, and that the law of Newton corresponds in fact to a zero density (see also (Poisson, 1833)). Poisson might have thus sensed the possibility of still other forces, besides those going inversely with the square of distance, corresponding to nonzero density of matter. Only after the work of Gauss became it gradually clear that the force inside matter should be taken first and foremost as a flux, and therefore expressed by its divergence, rather than by its curl as in mechanics of a single material point. And this divergence has as *expression the Newtonian density of matter*. However, in this approach the matter has to have the essential property of vacuum, which turns out to be the homogeneity with respect to space, in order to be possible to correctly characterize it by a density. This desideratum is, nevertheless, far from being satisfied with no further qualifications, for the homogeneity is a matter of scale. As Einstein says somewhere, the universe is homogeneous only 'on average'. The physics of last century added to this the essential observation that the property of homogeneity 'on average' should be respected *at any scale*.

Indeed, 'on average' the density of matter is never zero, not even hypothetically. Although we can imagine some smearing out procedure in order to calculate a density, that doesn't mean that we hit the real thing. As a matter of fact, the evaluations of the density of matter in universe taken today into consideration as scientific figures, don't even represent the Newtonian density as required by the Poisson's equation, but numbers obtained from various rough evaluations, with the substantial contribution of some numerical densities in the sense of Hertz (Hertz, 2003). These are combined with even more arbitrary evaluations of the volume of space where evaluations are made, assuming, still quite arbitrarily, that the matter should have a certain constitution in those regions of space. This is also the manner of evaluation of density for all the analyses related to the case of Sagittarius A*. However, with so many uncertainties in our hands, one can hardly think of a right quantitative appreciation of the density of matter! Useless to say, the very same is the case of evaluation of any density to be used into Poisson's equation.

5. Back to the General Newtonian Forces

We can see, therefore, that the development of differential calculus gradually spirited away the identity of force so to speak, *i.e.* the physical parameters representing the orbit from the expression of the magnitude of force.

Indeed, the force could now be calculated as a solution of a differential equation in satisfactory limiting conditions. The force thus became a plain vector. And the most natural among the analytical conditions a force vector should satisfy, when referring it to a continuum, seem to be the classical ones, generalizing the properties of the Newtonian force from Eq. (13), which show that it *acts in vacuum* and *is conservative*:

$$\nabla \cdot \vec{f} = 0; \quad \nabla \times \vec{f} = \vec{0} \tag{24}$$

In fact, at some moment, the classical theory of forces even stipulates specifically that a certain force vector can be split into a sum of a divergence-free part and a curl-free part – the so-called *Helmholtz decomposition* – and that the decomposition is unique. The conditions (24) legalize, so to speak, the two essential properties of the Newtonian gravitational force, only implicitly contained in the Poisson equation. The first condition says that the source of forces is the Newtonian density, but a vacuum force, like the Newtonian gravitational force, has no source; the second condition shows that the force is central, therefore conservative.

Let's say that we have obtained a formula for the magnitude of force in vacuum. The essential condition in order to be able to even use that formula is obviously that the force should satisfy the first Eq. (24). The second condition is only incidental, so to speak. However, if the magnitude of the force should depend exclusively on distance, then both conditions *are satisfied only for the Newtonian force* with magnitude inversely proportional with the square of the distance. Indeed, a central force with the magnitude depending exclusively on distance can be written in the form

$$\vec{f}(\vec{r}) = f(r)\frac{\vec{r}}{r} \tag{25}$$

where $f(r)$ is the magnitude of force. The second condition from Eq. (24) is automatically satisfied, while the first condition amounts to

$$rf'(r) + 2f(r) = 0 \quad \therefore \quad f(r) = \frac{\mu}{r^2} \tag{26}$$

Here the accent denotes the derivative with respect to the variable. Now it becomes obvious that the central forces inside matter, with magnitude depending exclusively on distance, require also a certain behavior of the density of matter depending on that distance, otherwise it is not a possible force whithin matter. Such a property is hard to understand geometrically, but is easy to understand… parametrically, as it were. More specifically, it is hard to

understand that a continuum has density decreasing in the same way in every direction starting from each one of its points. This would mean contradiction indeed, when we consider two different neighboring points. It is very easy to understand though, that a continuum has a certain density depending on the *distance between its points*, in cases where this distance can be defined.

However, if a force is central – therefore Newtonian – and has the magnitude dependent not only on distance but on direction too, then instead of Eq. (25) we must have

$$\vec{f}(\vec{r}) = \psi(x, y, z)\vec{r} \tag{27}$$

where *x, y, z* enter the expression of the magnitude of force by some algebraical combinations, other than the magnitude of the radius vector. In such a case the two conditions (24) boil down to

$$\sum x\frac{\partial \psi}{\partial x} + 3\psi = 0; \quad \vec{r} \times \nabla \psi = \vec{0} \tag{28}$$

Therefore the function ψ must be a homogeneous function of degree (–3), in the first place. If we limit our search to the functions derivable from the elliptic orbits of the planets, as Newton actually did, then such a function cannot be but of one of the following forms, also derivable from the second principle of dynamics (Darboux, 1877):

$$(\vec{a} \cdot \vec{r})^{-3}; \quad (a_{ij}x^i x^j)^{-3/2} \tag{29}$$

Here the vector $\vec{a}$ and the entries of matrix a are arbitrary constants, the coordinates are considered as contravariant, and the summation convention is respected. The expressions of forces are defined up to a multiplicative constant. We recognize in these the forces deriving from the Corollary 3 of the Proposition VII of Newton's Principia. Enforcing on them the second of conditions (28), shows that the first case is impossible, because the vector $\vec{a}$ would then have to be null identically. The second case works only if the matrix a is a multiple of the identity matrix. But this shows that the force is simply the Newtonian gravitational one, with the magnitude inversely proportional with the square of the distance. We thus find the Newtonian force as a property of field, with no reference whatsoever to motion, once it is conditioned by Eqs. (24). As we already expressed it, the identity of orbit – and therefore of force itself – is lost. However, it comes back, only this time through the initial conditions serving to solve the differential Eq. (15).

The inference about the existence of such particular forces in a problem of astrophysics should therefore be conditioned by the fulfillment of conditions

(28), therefore of the conditions (24). Those conditions reduce the class of forces, as Eqs. (29) show it in the most general case. Only the existence of Keplerian orbits would guarantee that these forces depend exclusively on distance, and moreover that their magnitudes are inversely proportional with the square of distance. This is a condition plainly satisfied by all of the results in the Sagittarius A* case: it came to attention of the scientific community by the very specific stellar orbits in the first place! And as Sagittarius A* is always in one of the foci of these orbits, which are of course elliptical, there can be no question of the reality of Newtonian force (13) in this case. Provided, of course, the matter exists in that place, *which is what the assumption of the existence of a black hole there brings about*. We are not quite so sure as to what extent, and in what particular conditions, the Kepler's second law, in its differential form, is satisfied for each one of those orbits. For, within Newtonian ideas, only the second of Kepler laws would be a clear indication of the presence and location of a center of force. As it happens though the theory of Newtonian forces works regardless of that law, and the conclusions of the present work should therefore remain theoretically valid (see (Mazilu, 2010; Mazilu and Agop, 2012)).

6. The Variation of Orbit and the Production of Fields

One of the main reasons for which we must appeal to the original Newtonian theory of forces in problems of astrophysics, like the one presented by the Sagittarius A* case, is that such a theory uses, almost explicitly we should say, an analogy which transcends the space scale of the problems in which this kind of forces is involved. The initial analogy was the one already mentioned in passing before, between sling shooting and the motion of planets. Then, with the gradual introduction of classical dynamics, the Eq. (15) made its entrance into the mathematics related to mechanics. And as long as we consider this equation as fundamental, one can prove that the force given by Eq. (13) is the only one justified from the point of view of space scale transcendence. Indeed, the Eq. (15) transcends the space scale, and no other force introduced in it satisfies this condition (Mariwalla, 1982). Therefore we are entitled to use the classical dynamics in describing the central part of the Milky Way just as we are entitled to use it in the case of describing planetary motions, or to state that the the stars move around the galactic nucleus following Keplerian orbits. It is at this juncture though, that we need to pay close attention to the concept of force to be used in astrophysical matters, for it might indicate some other fundamental things if it is to consider the point of view of *space scale transcendence*.

One historically important fundamental space scale transcendence is that allowing us to extend the conclusions of classical dynamics in the atomic realm. This means that the planetary – or nuclear – model of atom should be the only one entitled to close consideration from a theoretical physical point of view. This was indeed the case. Only, on this occasion we have learned that in

the microscopic realm the model does not work the same way as the planetary system proper. For, the light gets in: as long as electromagnetic phenomenon it should be attached to the atom, due to the electrical properties of this last one. It is here the point where the contradictions started brewing, forcing us to assign the light to *the transitions between electronic orbits* (Bohr, 1913). While the original Bohr's work is refering to the simplest atomic model – the one for which the electronic orbit is a circle – there are strong reasons to believe that his conclusion is quite general: the light or, in general, any perturbation that can reach our eyes directly or through the intermediary of measurement devices, *is due to transitions between orbits*. The arms of spiral galaxies can thus be interpreted as geometric loci of such transitions points (Mazilu, 2010; Mazilu and Agop, 2012), whereby the stars, revolving along Keplerian orbits around galactic nucleus, conglomerate in stable structures.

Therefore, through the planetary model of atom, theoretical physics actually just enacted a status quo, naturally existing a priori by the space scale transcendence. However, by Bohr's postulates, it is quite precise in the choice of the terms of analogy so to speak: the atomic model from microcosmos is analogous to the galaxy from macrocosmos, rather than to the planetary system per se. And by this, theoretical physics reinstated with full right the initial Newtonian forces, identified by the parameters representing the orbit from which they have been calculated. One might say that quantum mechanics of the atom was just a reaction of natural philosophy, which reclaimed the lost identity of the orbit in the expression of forces, or the lost identity of forces given by the orbit from which it was calculated.

7. The Characteristic of Forces Transcending Mechanics

The second of conditions (24) precludes the Newtonian forces from transcending mechanics, for it is equivalent with the conservation of mechanical energy, to the extent this is equivalent to work. The general Newtonian forces do not have this restriction: *they are dissipative*. For instance, the force characterizing a material point describing a Kepler orbit is given, according to Glaisher, by Eq. (5). Without any loss of generality, it can be written in vector form as

$$\vec{f}(x,y)=\frac{\mu\vec{r}}{\left(a_{13}x+a_{23}y+a_{33}\right)^{3}} \tag{30}$$

where (x,y) are the coordinates in the plane of motion. This force is of the form given in Eq. (29) with an obvious identification of function ψ, and for $a_{33} = 0$, in order to be considered a vacuum force. The general expression independent of the plane of motion is obviously the one using the first expression (29):

$$\vec{f}(x,y,z)=\frac{\mu\vec{r}}{\left(\vec{a}\cdot\vec{r}\right)^3}\quad\therefore\quad\psi(x,y,z)=\frac{\mu}{\left(\vec{a}\cdot\vec{r}\right)^3}\tag{31}$$

The first condition (29) is implicit, while the second condition is no more satisfied. In fact, we have

$$\nabla\times\vec{f}=-3\mu\frac{\vec{a}\times\vec{r}}{(\vec{a}\cdot\vec{r})^4}\tag{32}$$

Therefore, the elementary work of this force is not integrable in the ordinary sense. However it is integrable in the Frobenius sense, therefore in the thermodynamical sense, *i.e*. we have

$$\delta L\equiv\vec{f}\cdot d\vec{r}=wdF\tag{33}$$

for a certain functions *w* and *F*. This can be proved directly by noticing that the Cartan integrability condition $\delta L\wedge\lim_{x\to\infty}\left(d\wedge\delta L\right)=0$, where '$\wedge$' is the sign of an 'exterior' operation (in this case differentiation) on differential forms, is satisfied in view of Eqs. (31) and (32).

The classical motion sustained by the force from Eq. (31) is a Keplerian motion. This can be seen by solving the Binet's equation of the Newtonian problem of motion

$$u''+u=\frac{\mu/a^3}{\cos^3\theta}\tag{34}$$

where $u\equiv 1/r$ as usual, and the derivative is taken with respect to angle θ whose origin is the direction of the vector $\vec{a}$. The general solution of this equation

$$u(\theta)=(w_1-\mu/a^3)\cos\theta+w_2\sin\theta+\frac{\mu/2a^3}{\cos\theta}\tag{35}$$

where w_1 and w_2 are some initial conditions of the problem. In the Cartesian coordinates ξ and η with respect to the center of force Eq. (35) becomes

$$(w_1-\mu/2a^3)\xi^2+w_2\xi\eta+(\mu/2a^3)\eta^2-\xi=0\tag{36}$$

The center of the orbit has the coordinates

$$\xi_c=\frac{\mu a^3}{2w_1\mu a^3-w_2^2a^6-\mu^2};\quad\eta_c=\frac{w_2a^6}{2w_1\mu a^3-w_2^2a^6-\mu^2}\tag{37}$$

Therefore the physical parameters entering the force – the components of the vector $\vec{a}$ – determine also the characteristics of the Keplerian orbit induced by that force. This orbit is plane, with the plane determined by the initial conditions represented by the vector $\vec{w}$. The work of the force performed on the orbiting body is not zero, as in the case of the forces with magnitude depending exclusively on distance, but can be recognized by a flux through the surface enclosed by the orbit, for we have

$$\oint_{Orbit} \vec{f}(\vec{r})\cdot d\vec{r} = \iint_{Surface} (\nabla\times\vec{f})\cdot d\vec{S} = -3\mu\iint_{Surface} (\vec{a}\cdot\vec{r})^{-4}(\vec{a}\times\vec{r})\cdot d\vec{S} \quad (38)$$

What, though, if the orbit is not is not a closed curve?! In the Sagittarius A* case, for instance, all the data we have at our disposal, except the one referring to S02, come only with segments of the whole orbit. Therefore, such data would only refer to the work done by force along an open segment of the orbit, and the proper question would be the to ask about the variation of this integral along the orbit. A solution to this problem is provided by the transport theorem (Betounes, 1983) in the form

$$\frac{d}{dt}\int_{\varphi_t(\Gamma)} \vec{f}\cdot d\vec{r} + \int_{\varphi_t(\Gamma)} [(\nabla\times\vec{f})\times\vec{v}]\cdot d\vec{r} = \vec{f}\cdot\vec{v}\Big|_Q^P \quad (39)$$

Here we have a subtle understanding of things: Γ is the segment of curve initially accessible. It evolves due to the motions of heavens – not only of the body on which we have concentrated our attention. The evolution is accounted for by a family φ_t of morphisms depending on time in the sense that time is a continuous index of the family: for each moment of time there is a morphism mapping the initial segment Γ, between points *P* and *Q* of the orbit, to the current one denoted $\varphi_t(\Gamma)$. The Eq. (39) can be reckoned as a continuity equation, showing how the power generated by force is dissipated.

In the particular case of Eq. (32) we have

$$\frac{d}{dt}\int_{\varphi_t(\Gamma)} (\vec{a}\cdot\vec{r})^{-3}(\vec{r}\cdot d\vec{r}) - 3\vec{a}\times\int_{\varphi_t(\Gamma)} (\vec{a}\cdot\vec{r})^{-4}(\vec{r}\times\vec{v})\cdot d\vec{r} = (\vec{a}\cdot\vec{r})^{-3}(\vec{r}\cdot\vec{v})\Big|_Q^P \quad (40)$$

Because the motion is plane, the second term is zero, so that we are left with

$$\frac{d}{dt}\int_{\varphi_t(\Gamma)} (\vec{a}\cdot\vec{r})^{-3}(\vec{r}\cdot d\vec{r}) = (\vec{a}\cdot\vec{r})^{-3}(\vec{r}\cdot\vec{v})\Big|_Q^P \quad (41)$$

which means

$$\frac{d}{dt}\left\{(\cos\theta)^{-3}\int_{\varphi_t(\Gamma)} r^{-2}dr\right\} = \frac{v\cos\alpha(\theta)}{r^2(\cos\theta)^3}\Bigg|_Q^P \tag{42}$$

where $\alpha(\theta)$ is the angle between the current position vector and the current velocity vector.

In case we use the geometry to identify the displacement with the velocity, instead of (37) we must have

$$\frac{v_x}{-(a_{12}x+a_{22}y)} = \frac{v_y}{a_{11}x+a_{12}y} \tag{43}$$

so that Eq. (36) becomes

$$(rot\vec{f}\times\vec{v})\cdot d\vec{r} = 3\mu\frac{(a_{11}x+a_{12}y)y-(a_{12}x+a_{22}y)x}{\left(a_{11}x^2+2a_{12}xy+a_{22}y^2\right)^4}\cdot \\ \cdot d(a_{11}x^2+2a_{12}xy+a_{22}y^2) \tag{44}$$

Both the Eqs. (38) and (44) show that when the orbit is a circle, the dissipative term is zero: in order to have dissipation the elliptical orbit is a necessity!

A rational approach of the problem of Newtonian forces is that where one accepts that the centripetal force exists in heavens, but it is submitted strictly to the third principle of dynamics. Therefore the centripetal force cannot be calculated but only from the centripetal acceleration, it is not the Newtonian force. This principle leads to reasonable results. Indeed for the conic section from Eq. (1), referred to its center, the curvature vector defined as usual by

$$\vec{k} = k\hat{n};\quad k \equiv \frac{f_{xx}f_y^2 - 2f_{xy}f_xf_y + f_{yy}f_x^2}{\left(f_x^2+f_y^2\right)^{3/2}} \tag{45}$$

has the magnitude

$$k = -\frac{a_{33}\Delta}{\left(\langle x|\mathbf{a}^2|x\rangle\right)^{3/2}} \tag{46}$$

Now, the centripetal acceleration is given by the general expression

$$kv^2 \equiv -\frac{a_{33}\Delta v^2}{\left(\langle x|\mathbf{a}^2|x\rangle\right)^{3/2}} \tag{47}$$

Here v is the magnitude of the tangential velocity, common to both the orbit and the oscullating circle. As the magnitude of the tangent velocity as given by Eq. (43) should be

$$v^2 \propto \langle x|\mathbf{a}^2|x\rangle \tag{48}$$

the magnitude of the pure centripetal force becomes

$$f = K\frac{\Delta}{\left(\langle x|\mathbf{a}^2|x\rangle\right)^{1/2}} \tag{49}$$

One can see that in the special case in which the orbit is a circle, the centripetal force is inversely proportional with the radius of the circle, as it should be. This is actually the long distance force used by Sciama to justify the universal inertia.

A little discussion on the importance of the tangent dynamics – the hamiltonian dynamics here. If the velocity from Eq. (43) is also the unique velocity of the material point in universe. then its components must be taken as the time derivatives of the coordinates, and the equations of motion are the Hamilton equations

$$|\dot{x}\rangle = \mathbf{I}\mathbf{a}|x\rangle; \quad \mathbf{I} \equiv \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \tag{50}$$

This is the essential idea of the theory of constraints! In general though, we need to take for the velocity

$$|v\rangle = \mathbf{I}\mathbf{a}|x\rangle \tag{51}$$

and the condition of tangency still needs explanation. This is the general problem of Newton: what are the possible orbits in a point of one of them, taken as reference orbit? In other words, what are the orbits in a point, corresponding to the same velocity vector? The Eq. (51) shows that they are given by the differential equation

$$d(\mathbf{a}|x\rangle) = |0\rangle \quad \therefore \quad (d\mathbf{a})|x\rangle + \mathbf{a}|dx\rangle = |0\rangle \tag{52}$$

which is, in fact an evolution law. In case the orbit is not a parabola, this equation of evolution can be written as an equation of motion for coordinates:

$$|dx\rangle = -\mathbf{a}^{-1}(d\mathbf{a})|x\rangle \tag{53}$$

What is the meaning of this evolution? Let's assume that the orbit varies, therefore the quadratic form defining it varies. This variation implies both the variation of the vector and the variation of the matrix, so that we must have

$$d\left\langle x\middle|\mathbf{a}\middle|x\right\rangle = \left\langle dx\middle|\mathbf{a}\middle|x\right\rangle + \left\langle x\middle|d\mathbf{a}\middle|x\right\rangle + \left\langle x\middle|\mathbf{a}\middle|dx\right\rangle \tag{54}$$

Using now the Eq. (53), shows that the variation of the quadratic form is only dictated by the variation of its coefficients:

$$d\left\langle x\middle|\mathbf{a}\middle|x\right\rangle = -\left\langle x\middle|d\mathbf{a}\middle|x\right\rangle \tag{55}$$

Moreover, if one takes even the quadratic form from Eq. (25) as it is, viz. nonhomogeneous, then its variation is given by

$$d\left\langle x\middle|\mathbf{a}\middle|x\right\rangle = -\left\langle x\middle|d\mathbf{a}\middle|x\right\rangle - 2\left\langle a_3\middle|\mathbf{a}^{-1}d\mathbf{a}\middle|x\right\rangle + 2\left\langle da_3\middle|x\right\rangle \tag{56}$$

Now one can see that this variation has a certain form for a certain evolution of the center of force itself. If, for instance, one takes

$$\left|da_3\right\rangle = (d\mathbf{a})\mathbf{a}^{-1}\left|a_3\right\rangle \tag{57}$$

then the variation of the quadratic form reduces to the variation of the coefficients as before.

One can therefore guess that there is a certain correlation between the motion of the center of force and the motion of the current (material) point along an orbit. It is like, if the current point on the orbit describes a Ptolemaic epicycle, the center of force must describe a conic, which shrinks or extends in dimensions as the motion along the orbit proceeds. The problem would then be to find the correlation between the two 'epicycles'. In the classical case one talks about the motions of the material components around the common center of mass.

Condition (57) expresses the fact that the family of conics described by the variation of the parameters is a family having the same center. Indeed, the equation of the center of the conic (25) is

$$\left|a_3\right\rangle + \mathbf{a}\left|x_c\right\rangle = \left|0\right\rangle \tag{58}$$

Now, if the center is fixed, then we have by differentiation:

$$\mathbf{a}^{-1}\left|da_3\right\rangle + (d\mathbf{a}^{-1})\left|a_3\right\rangle = \left|0\right\rangle \tag{59}$$

Expanding this equation gives the Eq. (57). Here we need to always remind that in solving Eq. (57) we don't necessarily have the null initial condition, but this is given by (58) whereby the initial values of the entries of a are the values corresponding to the current orbit, where the differentiation is performed. Onbly in case (0, 0) are the coordinates of the center of current orbit one can have null initial condition, but this is in general just a convention.

The classical theories are usually focused on the idea of the same center of force, according to which the geometrical center of the orbit varies. The best known example is that of the perihelion rotation. The equation of evolution of the center of orbit over the family is in this case the Eq. (59) above. There is therefore a duality here: a family of orbits of the same geometrical center is described by an evolution of the center of force, while a family of orbits of the same center of force is described by an evolution of the geometrical center. The orbits of the same geometrical center are then apt to describe, for instance, motions inside the extended attractive body (the Sun, the Earth, etc), while the orbits of the same center of force are apt to describe motion inside the extended attracted body (the Earth, the Moon, etc.). Nevertheless, the center of force, as well as the geometrical center, have similar behavior from a kinematical point of view. The difference between the two descriptions cannot come but from the fact that the two bodies have different physical properties, like viscosity for instance.

8. Conclusions

Many astrophysicians argue for the existence of a supermassive black hole at the center of Milky Way, in the location of the radio source Sagittarius A*. In our opinion the evidence suggest just the opposite.

While the observational data on the orbits of the starry objects around Sagittarius A*, being of a projective character, are entirely reliable, their physical explanation uses quite a particular type of Newtonian forces, namely those with magnitude depending exclusively on the distance between bodies. This limitation assumes a priori that the bodies connected by such forces are special material points, viz. space positions endowed with mass. At space scales such as that of the galactic center region in discussion, this assumption is not realistic, and therefore, implicitly, such particular forces are themselves not quite realistic. Still using Newtonian forces in argument, strongly suggested by observational data as a matter of fact, one should allow, on such an occasion, their full generality. This means that we only need to assume that they are central forces with no other further constraints.

Within the framework of the Newtonian theory of forces this freedom has important theoretical consequences discussed at length in the sections above. Among these consequences, maybe the most important one, from an astrophysical point of view, is that the presence of a supermassive black hole in

the center of Milky Way might not be a sustainable assumption. Moreover, if we look at the fact that not all scientists agree with the current definition and essential characteristics of a black hole (Hawking, 2014): "It has been suggested that the resolution of the information paradox for evaporating black holes is that the holes are surrounded by firewalls, bolts of outgoing radiation that would destroy any infalling observer. Such firewalls would break the CPT invariance of quantum gravity and seem to be ruled out on other grounds. A different resolution of the paradox is proposed, namely that gravitational collapse produces apparent horizons but no event horizons behind which information is lost. The absence of event horizons mean that there are no black holes - in the sense of regimes from which light can't escape to infinity. There are however apparent horizons which persist for a period of time. This suggests that black holes should be redefined as metastable bound states of the gravitational field. It will also mean that the CFT on the boundary of anti deSitter space will be dual to the whole anti deSitter space, and not merely the region outside the horizon."

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SAGITTARIUS A*: UN ARGUMENT ÎMPOTRIVA EXISTENȚEI UNEI GĂURI NEGRE ÎN CENTRUL CĂII LACTEE

(Rezumat)

Literatura din domeniul astrofizicii a încercat să contruiască un argument pentru existența unei găuri negre supermasive în centrul Căii Lactee, în locația sursei radio Sagittarius A*. În opinia noastră, folosind argumente de aceeași natură, dovezile existente arată exact contrariul. Astfel, în timp ce datele observaționale despre orbitele obiectelor stelare din jurul lui Sagittarius A*, având un caracter proiectiv, prezintă încredere, explicația lor fizică se bazează pe o categorie aparte de forțe Newtoniene, și anume acelea pentru care tăria lor depinde exclusiv de distanța dintre corpuri. În primul rând, această limitare presupune a priori faptul că aceste corpuri conectate de forțele în cauză sunt puncte materiale speciale, sau altfel spus sunt poziții în spațiu cu masă. La scări spațiale precum cea a centrului galactic în discuție, această presupunere nu este realistică și, prin urmare, în mod implicit, aceste forțe particulare nu sunt ele însele destul de realiste. Păstrând raționamentul acestor forțe Newtoniene, sugerate de fapt de datele observaționale, ar trebui, în acest caz, să acceptăm caracterul lor general. Prin urmare, trebuie doar să presupunem că acestea sunt forțe centrale, lipsite de orice alte constrângeri. Această libertate are importante consecințe teoretice în cadrul teoriei Newtoniene a forțelor, consecințe ce sunt discutate în prezenta lucrare. Printre acestea, cea mai importantă, din punctul de vedere al astrofizicii, este aceea că prezența unei găuri negre supermasive în centrul Căii Lactee poate să nu fie o presupunere sustenabilă. O alternativă este prezentată.

BULETINUL INSTITUTULUI POLITEHNIC DIN IAŞI
Publicat de
Universitatea Tehnică „Gheorghe Asachi” din Iaşi
Volumul 64 (68), Numărul 2, 2018
Secţia
MATEMATICĂ. MECANICĂ TEORETICĂ. FIZICĂ

HEUN SOLUTIONS' CLASS FOR AN EXTENSION OF KOMPANEETS KINETIC EQUATION

BY

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Received: May 18, 2018
Accepted for publication: June 11, 2018

Abstract. An extended Kompaneets equation has been theoretically investigated. Closed form stationary solutions have been derived in terms of Heun confluent functions. These functions are governing the distribution of scattered photons.

Keywords: Heun confluent functions; extended Kompaneets equation; relativistic corrections; photon' spectrum; Compton scattering.

1. Introduction

Intensive studies over the interaction between radiation and electrons through the Compton scattering processes reveal a rich and very exciting evolutions of both the photon spectrum and the involved electrons. One may note that the comptonization process seen through a multiple scattering scenario is encountered at the level of relativistic corrections to the Sunyaev-Zeldovich effect (Taylor and Wright, 1989) which are revealing complex mathematical representation for the spectral distortion. When it comes to analyse mathematically the spectrum of the distorted radiation field it proves that one

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should deal with forms of Kompaneets equation, the most exciting for exploration being the corrective ones for the sake of relativistic effects.

In the last decades, with the help of SuZIE and MITO telescopes, a series of 16 clusters were observed at the level of higher frequencies (Rephaeli *et al*., 2005), where a significant intensity spectral change as a result of photon scattering by thermal electrons is to be recorded. Exact expressions for the relativistically photon intensity distortion are indispensible, most ardently when it comes to compute precise values of cluster and cosmological parameters.

In this study, we are mainly concerned in the correlation of the Kompaneets equation' extensions and its solutions in terms of Heun type ones. Nowadays, this topic being a fervent one, extensions on the Kompaneets equation to the relativistic regime having an outstanding role permitting, for instance, a more accurate determination of spectral quantities in higher energetic regimes.

2. Spectral Distribution of Photons Dictated by Heun Confluent Functions

The dimensional nonlinear Kompaneets equation (Kompaneets, 1957), also known as the photon diffusion equation, has the above mathematical formulation,

$$\frac{\partial n}{\partial t}=\frac{1}{x^2}\frac{\partial}{\partial x}\left[x^4\left(\alpha n_x+\beta n+\gamma n^2\right)\right], \tag{1}$$

where $\alpha>0$, $\beta\geq 0$ and $\gamma>0$ define some arbitrary constants. The change of distribution function $n(x,t)$ is treated as a diffusion of photon-gas in the 'frequency space' along the frequency axis $x\equiv h\nu/kT_e$.

Eq. (1) models the Compton scattering type interaction between a low-energy homogeneous photon gas and a rarefied electron gas. A more physical configuration proposed also by Kompaneets for the equation of radiative transfer, applicable in case of Comptonization-hardening for the energetic severe condition $h\bar{\nu}\langle\langle kT_e\langle\langle m_ec^2$, is

$$\frac{\partial n}{\partial t}=\frac{kT_e}{m_ec^2}N_e\sigma_T c\frac{1}{x^2}\frac{\partial}{\partial x}\left[x^4\left(\frac{\partial n}{\partial x}+n+n^2\right)\right]. \tag{2}$$

It appears that Eq. (2) is no longer adequate within the frame of hard X-ray astronomy where the condition $h\bar{\nu}\rangle\rangle kT_e$ is often valid. In this case, using it would imply the presence a significant error in the final results.

A significant improvement of Eq. (2), under the much looser condition $kT_e \langle\langle m_e c^2$ and $h\nu \langle\langle m_e c^2$, has been deduced by D.B. Liu *et al*. in (Liu *et al*., 2004) by extending the Kompaneets equation

$$\frac{\partial n}{\partial t} = \frac{kT_e}{m_e c^2} N_e \sigma_T c \frac{1}{x^2} \frac{\partial}{\partial x} \left\{ x^4 \left(1 + \frac{7}{10} \frac{kT_e}{m_e c^2} x^2 \right) \left[\frac{\partial n}{\partial x} + n(1+n) \right] \right\}. \quad (3)$$

In the study of Sazonov and Sunyaev (Sazonov and Sunyaev, 2000), various elaborated generalized forms of kinetic equation which consider a density of correction terms responsible, for instance, for quantum effects, induced scattering or Doppler effect, have to be found. Relativistic corrections present within these versions of Kompaneets equation may play a significant role in problems such as the formation of shock waves in the photon spectrum during the phenomenon of Bose condensation of photons (Zeldovich and Sunyaev, 1972) or plasma heating (Levich and Sunyaev, 1971).

Within our study, following an analytical approach, we will focus on finding closed form solutions for the following extension of the Kompaneets equation:

$$\frac{\partial n}{\partial t} = \frac{1}{x^2} \frac{\partial}{\partial x} \left\{ x^4 \left(1 + ax^2 \right) \left[bx \frac{\partial n}{\partial x} + n(1+n) \right] \right\} \quad (4)$$

We mention that our class of extended Kompaneets equation, namely Eq. (4), is similar to the one proposed by Liu and coworkers, with the single distinction, the one that the Doppler term is being attended by a pre-factor.

Within the hypothesis of stationary, this equation is reduced to the Riccati type form

$$bx \frac{\partial n}{\partial x} + n + n^2 = \frac{Q}{x^4 \left(1 + ax^2 \right)} \quad (5)$$

with Q, as we find in (Dubinov, 2009), defining a constant whose physical meaning is of the photon flux in the implied frequency domain. The Riccati types equations are frequently encountered within the Kompaneets studies where these are discussed in detail.

In order to solve Riccati form (5), firstly we will invoke the change of variable $y = (1/b) \ln x$ which leads to the new representation

$$\frac{\partial n}{\partial y} + n + n^2 = \frac{Q}{e^{4by} \left(1 + ae^{2by} \right)}. \quad (6)$$

At this step, the change of function given by

$$n = \frac{\Psi'}{\Psi} \tag{7}$$

provides us with a second order differential equation for the function Ψ:

$$\Psi'' + \Psi' - \frac{Q}{e^{4by}\left(1+ae^{2by}\right)}\Psi = 0 \tag{8}$$

A new change of function given by $\Psi = \exp\left[-\frac{\sqrt{Q}e^{-2by}+2by}{2b}\right]\cdot u(y)$ leads to the following differential equation for the unknown function $u(y)$:

$$\begin{aligned}&\frac{d^2u}{dy^2}+\left(2\sqrt{Q}e^{-2by}+1\right)\frac{du}{dy}+\\&+\left(-2b\sqrt{Q}e^{-2by}+e^{-4by}Q+\sqrt{Q}e^{-2by}-\frac{Q}{e^{4by}\left(1+ae^{2by}\right)}\right)u=0\end{aligned}, \tag{9}$$

the solution of this equation being given by

$$u(y) = e^{-y}\,HeunC\left[\frac{a\sqrt{Q}}{b},\frac{1}{2b},-1,-\frac{a^2Q}{4b^2},\frac{1}{2},-\frac{e^{-2by}}{a}\right] \tag{10}$$

so that we can deduce that

$$\Psi = x^{-1/b}\cdot\exp\left[-\frac{\sqrt{Q}}{2bx^2}\right]\cdot HeunC\left[\frac{a\sqrt{Q}}{b},\frac{1}{2b},-1,-\frac{a^2Q}{4b^2},\frac{1}{2},-\frac{1}{ax^2}\right] \tag{11}$$

This expression allows us to determine the intricate photon distribution function defined in (7) in terms of the *HeunC* functions,

$$n = \frac{\sqrt{Q}-x^2}{bx^3}+\frac{HeunC'}{HeunC}. \tag{12}$$

To be noted that the spectrum of the scattered photons is intimately dependent on the photon flux Q in the respective frequency region.

For practical calculations, it is more elegant and transparent to recall the polynomial representation of the Heun confluent function. Heun function, $HeunC[\alpha,\beta,\gamma,\delta,\eta,z]$, admits a polynomial representation when the series expansion for it truncates, so that in this situation the function degenerates into a polynom. In our case, by invoking the algebraic constriction (necessary, but not sufficient) for this to happen, namely

$$\delta = -\left(n + \frac{\gamma+\beta+2}{2}\right)\alpha, \tag{13}$$

the identified parameters in (12) makes us obtain the relation

$$\frac{a\sqrt{Q}}{4b} = n + \frac{2b+1}{4b} \tag{14}$$

which is equivalent with the following parametric constriction

$$a\sqrt{Q} = 4nb + 2b + 1. \tag{15}$$

To be noted that n is a positive integer defining the polynom' degree.

For more insights into polynomial representations, we recommend the study in (Fiziev, 2010) where it is to be found an innovative derivation of confluent Heun's polynomials.

As Heun functions are mathematically difficult to operate with, due to the singularities or to their problematic act of derivation a series, their polynomial forms are very useful. These allow a compactified and a more tractable representation.

3. Conclusions

Within an analytical approach, closed form solutions for a relativistically corrected Kompaneets equation have been determined. The spectrum of the scatterred photons proved to be non-trivially determined by the Heun confluent functions and intimately connected with the photon flux in the respective frequency domain. The polynomial Heun solution has been discussed in terms of parametric constriction.

Acknowledgements. This work was supported by a grant of Ministery of Research and Innovation, CNCS-UEFISCDI, project number PN-III-P4-ID-PCE-2016-0131, within PNCDI III.

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CLASA DE SOLUȚII HEUN PENTRU O EXTENSIE A ECUAȚIEI CINETICE KOMPANEETS

(Rezumat)

O formă extinsă a ecuației Kompaneets a fost investigată teoretic. Au fost determinate soluții staționare în formă închisă, exprimate prin funcții Heun confluente. Aceste funcții guvernează distribuția fotonilor împrăștiați. Soluția polinomială Heun a fost analizată în termenii constrângerii parametrice.

BULETINUL INSTITUTULUI POLITEHNIC DIN IAŞI
Publicat de
Universitatea Tehnică „Gheorghe Asachi” din Iaşi
Volumul 64 (68), Numărul 2, 2018
Secţia
MATEMATICĂ. MECANICĂ TEORETICĂ. FIZICĂ

ANISOTROPY IN INFLAMMATORY SYSTEMIC DISEASES – A THEORETICAL MODEL

BY

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Received: April 12, 2018
Accepted for publication: June 12, 2018

Abstract. Microbiota refers to the total microorganisms of the microbial community, while the term microbiome refers to a group of microbes that includes bacteria, bacteriophages, fungi, protozoa and viruses. Microbiota is considered to be an organ with its own functions that can modulate the expression of genes involved in the defense of mucosal barrier, angiogenesis and postnatal intestinal maturation. Changes in the composition of gut microbiota, *i.e.* dysbiosis, may be associated with nosocomial infections, necrotizing enterocolitis in premature infants, inflammatory bowel disease (IBD), obesity, rheumatologic autoimmune diseases and allergies. Dysbiosis increases intestinal permeability and the microbial translocation through the mucosa, thus resulting in inflammation and metabolic endotoxemia. Therefore, a large number of proinflammatory cytokines and oxygen free radicals are generated, all of which are considered triggers for the development of immuno-inflammatory systemic diseases. Many clinical studies have examined the link between autoimmune diseases and dysbiosis using 16S rRNA genetic analysis. Clear evidences of association with intestinal dysbiosis have been described in patients diagnosed with IBD, spondylarthropathies, rheumatoid arthritis or systemic lupus erythematosus. A mathematical model based on group invariance is developed.

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Keywords: microbiota; intestinal dysbiosis; inflammatory bowel disease; spondylarthropathies; rheumatoid arthritis; systemic lupus erythematosus.

1. Introduction

Bacterial intestinal flora includes about 10^{14} bacteria which represents 10 times more than the number of cells in the human body (Arrieta *et al*., 2014; Saavedra and Dattilo, 2012). Since birth, the normal intestinal microbiota contributes to the development of intestinal function, modulates the immune system, helps to regulate and maintain intestinal function, provides protection against infection and tolerance to food intake. We can talk about a symbiosis of the bacteria-host interaction. Intestinal microbiota diversity includes more than 1,500 microbial species, dominant bacteria group being phyla species: Firmicutes and Bacteroidetes. The phyla group also includes: Proteobacteria, Actinobacteria, Fusobacteria and Verrucomicrobia (Human Microbiome Project C, 2012).

Microbiota has multiple roles in the development of the intestinal immune system by: the modulation of intestinal mucous layer and lymphoid structures, differentiation of immune cells and immune mediators production, positive stimulatory effect on the innate and adaptive immune system (Akira, 2006).

Changes in the composition of gut microbiota - dysbiosis - may be associated with nosocomial infections, necrotizing enterocolitis in premature babies, IBD, obesity, rheumatologic autoimmune diseases and allergies. Dysbiosis increases intestinal permeability and the microbial translocation through the mucosa, thus resulting inflammation and metabolic endotoxemia. Therefore, a large number of proinflammatory cytokines and free radicals are generated (Seksik and Langella, 2008).

Dysbiosis influence the intestinal mucosa by interacting with epithelial cells and by the enteric nervous system, leading to changes in intestinal motility, sensory function and the perception of pain (Konturek, 2011). Also, dysbiosis is associated with the development of gastrointestinal and extraintestinal disorders, as well as with an impaired liver function (Seksik and Langella, 2008; Mondot *et al*., 2013).

2. Microbiota and IBD

Genetics and environmental factors and the host immunity forms a triad that it has been shown to regulate the TCR function (Toll like receptor). When this relationship is disturbed, it can develop aberrant TCR signals which contribute to the formation of inflammasomes that will cause intestinal inflammation (IBD) (Frosali *et al*., 2015).

Risk factors for the occurrence of IBD include factors that influence the composition of intestinal microbiota - maternal exposure, breastfeeding, diet, antibiotics, infections and factors affecting mucosal immune system - smoking, NSAIDs, oral contraceptives, vaccination, intestinal permeability, appendectomy, stress (Danese *et al*., 2004). A model of colitis on laboratory mice showed that, after the administration of 4 antibiotics for 4 weeks, the deletion of commensal gut microbiota can cause severe intestinal mucosal impairment (Rakoff-Nahoum *et al*., 2004). Extended use of antibiotics is associated with increased risk of Crohn's disease (CD), but not with ulcerative colitis (UC) (Ungaro *et al*., 2014).

One study attempted to investigate the impact of IBD on intestinal microbiota being analyzed 89 sigmoid mucosal biopsies in healthy individuals and in patients with CD and UC who achieved remission. On these biopsy samples 16sDNA and rARN genetic analysis were performed. Results showed an abundance of Bacteroides in the control group and in patients with UC, an increase of Firmicutes in both IBD, a reduced activity of Faecalibacteria in patients with CD, an increase in the prevalence and activity of Papillibacter in healthy persons; only Prevotella was positively associated with CD (Rehman *et al*., 2015).

Dysbiosis in CD is characterized by: a greater number of mucosal bacteria compared to healthy individuals, alteration of the balance between beneficial and aggressive bacteria and by the reducing of the phyla diversity group Firmicutes and Bacteroides (Sartor, 2011). Increased prevalence of intracellular pathogens in CD may be due to the innate immune system's inability to control persistent infections caused by intracellular bacteria.

Patients with ileal and colonic CD have a low concentration of commensal bacteria concerning the Clostridiales group as Faecalibacterium prausnitzii and Roseburia (Willing *et al*., 2010), these being regarded as predictive marker for postoperative ileal CD (Sokol *et al*., 2008). An increased number of bacterial species found in CD include Escherichia coli especially B2 and D groups and those with adherent / invasive strains associated with a severe ileal disease (Kotlowski *et al*., 2007).

3. Microbiota and Inflammatory Rheumatic Diseases

Except reactive arthritis in which there are clear evidences that bacterial infections can cause articular manifestations, currently studies show only hypotheses regarding the role of gut microbiota in immune-mediated arthritis. However, a study conducted on mice having ankylosing spondylitis (AS) and positive antigen HLA-B27 and which were maintained in germ-free conditions highlighted that they didn't developed articular inflammation (Jacques and Elewaut, 2008).

Recent studies argue that, intestinal dysbiosis in patients with SA correlates with the presence of the antigen HLA-B27. To detect bacteria

associated to HLA-B27, 16S rRNA sequencing had been used and elevated populations of Paraprevotella and Bacteroides vulgatus have been highlighted (Lin *et al*., 2014). Altered intestinal bacterial composition characterized by: increasing populations of Lachnospiraceae, Ruminococcaceae, Rikenellaceae, Porphyromonadaceae, Bacteroidaceae, alongside the decreasing of Veillonellaceae and Prevotellaceae constitutes a risk factor for developing SA (Costello *et al*., 2015).

A recently published study supports the important role of intestinal dysbiosis (especially Dialister gender) in spondylarthropathies. There have been included 27 patients of which 14 showed microscopic intestinal inflammation and 13 without gut inflammation. Ileal and colonic biopsies were performed. 16SrARN sequences were used in order to compare the intestinal microbial composition. The results showed that the microbiota of patients with spondylarthropathies was associated with intestinal inflammation and Dialister gender was positively correlated with the ASDAS score (Ankylosing Spondylitis Disease Activity Score) (Tito *et al*., 2016).

Other diseases such as rheumatoid arthritis (RA) or systemic lupus erythematosus (SLE) may have as pathogenic mechanism intestinal dysbiosis which contributes to the development of arthritis through activation of autoreactive T cells in the gut (Maeda *et al*., 2016). Dysbiosis in RA is characterized by a depletion of Haemophilus spp. - negatively correlated with the level of autoantibodies - and an increasing of Lactobacillus salivarius - especially in cases of very high RA activity (Zhang *et al*., 2015). Regarding SLE patients, trials evidenced a significant decrease in Firmicutes and Firmicutes/Bacteroidetes ratio and a significant increase in Clostridiaceae and Lachnospiraceae groups that correlated with disease progression (Hevia *et al*., 2014).

4. Microbiota and IBD Associated with Articular Manifestations

Regarding the association between IBD and rheumatic disorders, namely AS, it must not forget that these conditions have common genetic background and are considered distinct phenotypes of an immune-mediated inflammatory disorder. The strongest genetic association is represented by the antigen HLA-B27.

Intestinal epithelial cells produce mucins and antimicrobial peptides such as lysozyme, defensins and lectins that have a critical role in intestinal homeostasis. Patients with active CD show a marked decrease of DEFA5 and DEFA6 α-defensins, leading to an impaired mucosal commensal microbial flora. Controversially, the studies showed an increased expression of α-defensins in patients with SA having also subclinical ileal inflammation (Wehkamp *et al*., 2005).

Regarding IL-17 / IL-22 cytokines relevant to IBD and spondylarthropathies, clear evidences indicate that the interaction between gut

microbiota and host causes the activation of immune cells with subsequent production of these types of proinflammatory cytokines (Shaw *et al*., 2012).

5. Mathematical Model

Inflammation results from the accumulation of multiple alterations in a single transformed tissue. Even if the probability of transformation is extremely low for a single tissue, inflammation could arise by chance within a lifetime if many tissue layers are at risk (see the above-mentioned risk factors). Many common inflammations exhibit an increase in incidence with age, which can be described by a simple equation:

$$p = bt^k$$

Parameters are *p* (probability of inflammation), *b* (a constant), *t* (age of individual), and *k* (the number of rate-limiting stages of inflammation). In a particular case, when the inflammation can be associated to cancer, the equation fits the epidemiology of colorectal cancer when *k* is 5 or 6.

This equation does not include many biological parameters, which are presumably incorporated into its constant *b*. Intuitively, inflammation incidence should increase with greater numbers of cells at risk, with greater numbers of cell divisions, and with higher mutation rates.

In this paper we present a simple algebraic equation that relates small biological features (adult stem cells and their niches, tissue size, numbers of rate-limiting driver mutations, and mutation rates) with the epidemiology of inflammatory diseases.

The probability of inflammation is 10^{-36} when the mutation rate (*u*) is 10^{-6} mutations per gene per division and *k* is six. It is highly improbable that inflammation will arise in a single cell after a single division. A more useful calculation is the probability of inflammation after the many divisions that occur during a human lifetime, and in just one of the many tissues at risk in the body. The approach is based on the trick that the probability of "something" plus the probability of "not something" equals one. The probability of not accumulating a critical mutation (1-*u*) in one cell lineage after a certain number of divisions (*d*) is:

$$p = (1-u)^d$$

With more divisions, the probability of no mutation decreases. It follows that the probability of mutation after d divisions is:

$$p = 1-(1-u)^d$$

For multiple (k) genes:

$$p = [1-(1-u)^d]^k$$

The above equation calculates the probability of a single cell accumulating all k driver mutations after d divisions. We must note that this model was developed in the case of isotropic inflammation.

In vivo, biological structures display, by their own nature, an anisotropic behavior. In this context, the following problem arises: can the above results be generalized to the anisotropic case?

In order to solve this problem, let us first make the following substitutions, in accordance with the one-dimensional model we developed:

$$\begin{aligned} &p = [1-(1-u)^d]^k \\ &p = x \\ &[1-(1-u)d]^k = y^2 \end{aligned}$$

It results that the inflammation probability law takes the form:

$$y^2 = x \tag{1}$$

The plane geometry associated to Eq. (1) can be founded on a parametric group which must make the form from relation (1) invariant. This group can be best revealed if the homogenous coordinates (y, x) are used in the form:

$$\frac{x_1}{x} = \frac{x_2}{y} = \frac{x_3}{1} \tag{2}$$

where

$$\begin{aligned} &x = [1-(1-u)^d]^k \\ &y = [1-(1-u)d]^{k/2} \end{aligned} \tag{3}$$

case in which Eq. (1) becomes:

$$x_2^2 - x_1 x_3 = 0 \tag{4}$$

In this situation, the conic from relation (4) accepts the canonic parameterization:

$$\frac{x_1}{t^2} = \frac{x_2}{t} = \frac{x_3}{1} \tag{5}$$

where t is a real parameter, and its invariance group is the three-parameters group generated by the homographic transformation of the t parameter. If this transformation is written under a more convenient form,

$$t = \frac{t + \alpha_1}{1 - \alpha_2 - \alpha_3}, \tag{6}$$

which highlights the unit transformation for $\alpha_1 = \alpha_2 = \alpha_3 = 0$, then using Eq. (5) the following transformation relations for the parameters x_1, x_2 result

$$\begin{aligned} x_1 &= \frac{x_1 + 2\alpha_1 x_2 + \alpha_1^2}{\alpha_3^2 x_1 - 2\alpha_3 (1 - \alpha_2) x_2 + (1 - \alpha_2)^2} \\ x_2 &= \frac{-\alpha_3 x_1 + (1 - \alpha_2 - \alpha_1 \alpha_3) x_2 + \alpha_1 (1 - \alpha_2)}{\alpha_3^2 x_1 - 2\alpha_3 (1 - \alpha_2) x_2 + (1 - \alpha_2)^2} \end{aligned} \tag{7}$$

from which a continuous two variables with three parameters group can be observed. The Lie algebra (Duistermaat and Kolk, 2000) is given by the operators:

$$\begin{aligned} L_1 &= 2y \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \\ L_2 &= 2x \frac{\partial}{\partial x} + y \frac{\partial}{\partial y} \\ L_3 &= 2xy \frac{\partial}{\partial x} + \left(2y^2 - x\right) \frac{\partial}{\partial y} \end{aligned} \tag{8}$$

with the commutation relations:

$$\begin{aligned} \left|L_1, L_2\right| &= L_1 \\ \left|L_2, L_3\right| &= L_3 \\ \left|L_3, L_1\right| &= -2L_2 \end{aligned} \tag{9}$$

where inhomogeneous coordinates were taken into account in order to simplify the writing.

As it should be, the conics in relation (4) appear in this situation as the Eq. (8) group's invariant varieties with two parameters, and this is why they are invariant only with regard to the first two operators from relation (8). The issue at hand is not to find the two-parameters invariant varieties families, but to find the three-axial that holds three parameters: the main inflammations, *i.e.* the eigenvalues of the inflammations tensor. Now the inflammations evolution group remains to be solved, which must be isomorphic to the group from Eq. (8). In order to highlight it we must note that the main inflammations are the solution to the secular equation of the respective matrix, which can be written as:

$$y^3 + 3a_1 y^2 + 3a_2 y + a_3 = 0 \tag{10}$$

where $3a_1, 3a_2, a_3$ are the orthogonal invariants of the inflammations matrix. If the inflammation state varies from y_1, y_2, y_3 to y'_1, y'_2, y'_3 then an algebra theorem (Burnside, 1960) shows that between the secular equations, which have the respective values as roots, a linear relation takes place, generated by the homographic transformation

$$y' = \frac{ay + b}{cy + d} \tag{11}$$

which gives a three-parameters group but in three variables. By writing the roots of the curve from relation (10) in the Barbilian form (Barbilian, 1967; Kelly, 1954),

$$y' = \frac{h + \varepsilon_i \bar{h} k}{1 + \varepsilon_i k} \tag{12}$$

where $\varepsilon_i^3 = 1$, $h, \bar{h}$ are quantities conjugated one to the other, and k is a one-module complex factor, the transformation from Eq. (11) induces upon the quantities $h, \bar{h}, k$ the real transformations

$$\begin{aligned} h' &= \frac{ah + b}{ch + d} \\ \bar{h}' &= \frac{a\bar{h} + b}{c\bar{h} + d} \\ k' &= \frac{c\bar{h} + d}{ch + d} k \end{aligned} \tag{13}$$

which form a three variables with three parameters group (Burnside, 1960), *i.e.* the Barbilian group.

This group is simple transitive, with the infinitesimal generators given by the operators:

$$\begin{aligned} A_1 &= \frac{\partial}{\partial h} + \frac{\partial}{\partial \bar{h}} \\ A_2 &= h \frac{\partial}{\partial h} + \bar{h} \frac{\partial}{\partial \bar{h}} \\ A_3 &= h^2 \frac{\partial}{\partial h} + \bar{h}^2 \frac{\partial}{\partial \bar{h}} + \left(h - \bar{h}\right) k \frac{\partial}{\partial k} \end{aligned} \tag{14}$$

which reveals for the associated Lie algebra a structure that is identical with the one from Eq. (9). Therefore, the two groups are isomorphic, the operators (8) and (14) being generated by the one and the same algebra (4). Moreover, the group (14), being simple transitive, is definitely measurable, its elementary measure being given by the differential three-form:

$$\frac{dh \wedge d\bar{h} \wedge dk}{\left(h-\bar{h}\right)^2 k} \tag{15}$$

As such, in the field variables space $\left(h,\bar{h},k\right)$ a probabilities theory can be apriori constructed using the elementary probability

$$dP = \frac{dh \wedge d\bar{h} \wedge dk}{\left(h-\bar{h}\right)^2 k}$$

As usual, the quadratic root of this function is defined up to an arbitrary unimodular factor, and it can be assimilated to the wave function analogue. Then, it will satisfy a Schrödinger type equation, equation which defines geodesics in a fractal space-time.

The issue now at hand is to find the invariant varieties families of the group (8) with three parameters, having group (14) associated as a parameters group. In our opinion these functions can provide for an answer to the problem of the correlation between the one-dimensional and three-dimensional behaviors of the inflammation.

These varieties families will be solutions of the Stoka (Stoka, 1968) equations:

$$\begin{aligned}
&2y\frac{\partial f}{\partial x}+\frac{\partial f}{\partial y}+\frac{\partial f}{\partial h}+\frac{\partial f}{\partial \bar{h}}=0\\
&2x\frac{\partial f}{\partial x}+y\frac{\partial f}{\partial y}+h\frac{\partial f}{\partial h}+\bar{h}\frac{\partial f}{\partial \bar{h}}=0\\
&2xy\frac{\partial f}{\partial x}+\left(2y^2-x\right)\frac{\partial f}{\partial y}+h^2\frac{\partial f}{\partial h}+\bar{h}^2\frac{\partial f}{\partial \bar{h}}+\left(h-\bar{h}\right)k\frac{\partial f}{\partial k}=0
\end{aligned} \tag{16}$$

This system admits solutions of the form:

$$f\left(\alpha,k_0^2\right)=\text{const.} \tag{17}$$

where:

$$\alpha = \frac{\sqrt{x-y^2}\left(h-\bar{h}\right)}{x-\left(h-\bar{h}\right)y+h\bar{h}}$$
$$k_0^2 = k^2\,\frac{x-2y\bar{h}+\bar{h}^2}{x-2yh+h^2} \tag{18}$$

It can be observed that the last of these integrals is a one-module complex one. In principle, f can be any function which is continuous and derivable in its variables. It is not yet known what kind of interpretation can a general solution such as Eq. (17) have, but some specific integrals values from relation (18) can still be interpreted. Thus, if the one-dimensional inflammation is monotonous, then Eq. (18) must fulfill the condition $y^2 = x$, fact which leads to the specific value $x = 0$. In this case, the second relation (18) gives:

$$k_0 = k\,\frac{y-\bar{h}}{y-h} \tag{19}$$

from which we can write y as:

$$y = \frac{\bar{h}k - hk_0}{k-k_0} \tag{20}$$

The result we obtained in this case is important mainly because it shows that y can be identified in a specific case with one of the main inflammations. Indeed, if $k_0 \equiv (-1, -\varepsilon, -\varepsilon^2)$ then the situation from Eq. (12) is again reached. Therefore, we can state that in both these specific cases the inflammation in the one-dimensional case can be considered as one of the internal inflammations eigenvalues. However, we can draw more from Eq. (20). If this equation is written for $k_0 = -1$,

$$y = \frac{h+\bar{h}k}{1+k} \tag{21}$$

and $h, \bar{h}, k$ are explicitly written with regard to the main inflammation, and also the system of Eqs. (12) is solved with regard to $h, \bar{h}, k$, then the following relations can be found:

$$h = -\frac{y_2y_3 + \varepsilon y_3y_1 + \varepsilon^2 y_1y_2}{y_1 + \varepsilon y_2 + \varepsilon^2 y_3}$$
$$k = \frac{y_1 + \varepsilon^2 y_2 + \varepsilon y_3}{y_1 + \varepsilon y_2 + \varepsilon^2 y_3} \tag{22}$$

These can be related with the above-mentioned parameters by:

$$k = -e^{3i\xi}$$
$$h = \lambda + \frac{\mu}{\sqrt{3}}\left(\sin 3\xi - i\cos 3\xi\right) \tag{23}$$

where

$$\tan\xi = \frac{2y_1 - y_2 - y_3}{\sqrt{3}\left(y_2 - y_3\right)}$$
$$\lambda = \frac{1}{3}\left(y_1 + y_2 + y_3\right) \tag{24}$$
$$\mu = \frac{1}{\sqrt{2}}\left\{\sum\left(y_2 - y_3\right)^2\right\}^{\frac{1}{2}}$$

The quantity from Eq. (24) is the known Lode-Nadai parameter of the tensions tensor.

If we use Eq. (23) in relation (21), we obtain the following:

$$y = \lambda + \mu\sin\xi \tag{25}$$

relation which, in the case of the absence of anisotropic inflammation, is reduced to:

$$y = \mu\sin\xi \tag{26}$$

From this it results that the one-dimensional inflammation can be identified with the quantity μ from Eq. (24) only if the inflammations which are orthogonal to the direction of disease expansion are very close to each other. Indeed, in this case, from relation (24) it results that $\tan\xi \to \infty$, and, thus, $\sin\xi \to 1$.

6. Conclusions

The main conclusions of the present paper are presented in the following:

i) The gut microbiota plays an important role in the development of immuno-inflammatory diseases, namely in intestinal and articular disorders. Nevertheless, the specifically pathogenic mechanism remain a challenge for the practitioner physician. The analysis of gut microbiota opens new perspectives in research and for understanding of these systemic diseases.

ii) Starting from an isotropic model, an anisotropic theoretical model is developed for inflammatory disease evolution.

We note that the same model can also be applied, because of its theoretical implications, in engineering and materials science, in various domains, such as the ones described in (Agape *et al*., 2016; Agape *et al*., 2017; Gaiginschi *et al*., 2011; Gaiginschi *et al*., 2014a; Gaiginschi *et al*., 2014b; Gaiginschi *et al*., 2017; Vornicu *et al*., 2017).

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ANIZOTROPIA ÎN BOLILE INFLAMATORII SISTEMICE – UN MODEL TEORETIC

(Rezumat)

Microbiota este considerată un organ cu funcții specifice, ce poate modula expresia genelor implicate în protejarea barierei mucoase, angiogeneză sau maturarea intestinală postnatală. Modificări ale compoziției microbiotei intestinale, numite într-un cuvând disbioză, pot fi asociate cu infecțiile nosocomiale, boala intestinală inflamatorie, obezitate, alergii etc. Disbioza mărește permeabilitatea instestinală și crește rata de mișcare microbiană la nivelul mucoasei, având ca rezultat endotoxemie inflamatorie și metabolică. Toate aceste cauze pot genera boli imuno-inflamatorii sistemice. Plecând de la aceste premise, în prezenta lucrare se construiește un model matematic bazat pe invarianță grupală, care permite extensia de la multiplicarea omogenă și izotropă la cea neomogenă și anizotropă, în cazul evoluției bolilor inflamatorii, cum de regulă se întâmplă în structurile biologice.

BULETINUL INSTITUTULUI POLITEHNIC DIN IAŞI
Publicat de
Universitatea Tehnică „Gheorghe Asachi” din Iaşi
Volumul 64 (68), Numărul 2, 2018
Secţia
MATEMATICĂ. MECANICĂ TEORETICĂ. FIZICĂ

QUANTUM MECHANICAL CHARACTERIZATION OF THYMOL BLUE

BY

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Received: May 28, 2018
Accepted for publication: June 13, 2018

Abstract. Thymol blue (TB) is an important acid basic color indicator used in various applications. Its parameters in the ground state are very important for applications, so a comparative study of physical parameters of TB was realized by three methods from Spartan 14, in order to establish the more convenient method to be used in our spectral applications.

After the geometrical optimization, the TB main parameters like length of the chemical bonds, charges near the component atoms, the dihedral angles, dipole moments, polarizability of this molecule were computed.

Keywords: thymol blue; atomic charges; dipole moment; polarizability.

1. Introduction

The molecule of 4-[3-(4-hydroxy-2-methyl-5-propan-2-ylphenyl)-1,1-dioxobenzo[c]oxathiol-3-yl]-5-methyl-2-propan-2-ylphenol also named thymol blue (TB) (Balderas-Hernandez, 2007) is formed by three benzene rings bonded to a central carbon, with a sulphonic group attached to one of the rings and keto-enol groups bonded to other rings (see the structural formula displayed in Fig. 1).

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The chemical formula of TB is $C_{27}H_{30}O_5S$, its molar mass is 466.592 g/mol, its melting point is 221-224°C and its flash point is 36°C. TB is a brownish-green or reddish-brown crystalline powder, insoluble in water but soluble in alcohol and dilute alkali solutions.

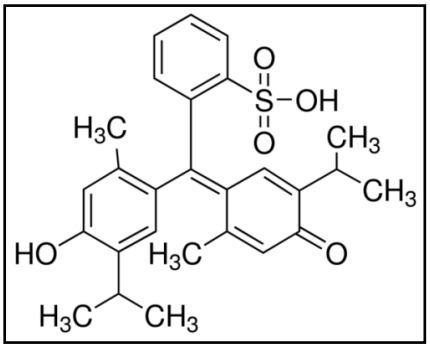


Fig. 1 – Structural formula of TB.

TB is an acid-base indicator from the family of sulphonephtalein, which has two color transition intervals, passing from red to yellow at pH 1.2 – 2.8 and from yellow to blue at pH 8.0 – 9.6 (Pub. Chem. Database https: pubchem ncbi.nlm.nih.gov, access 2018).

The purpose of this paper is to carry out a quantum-chemical study of the TB molecule to establish its molecular parameters.

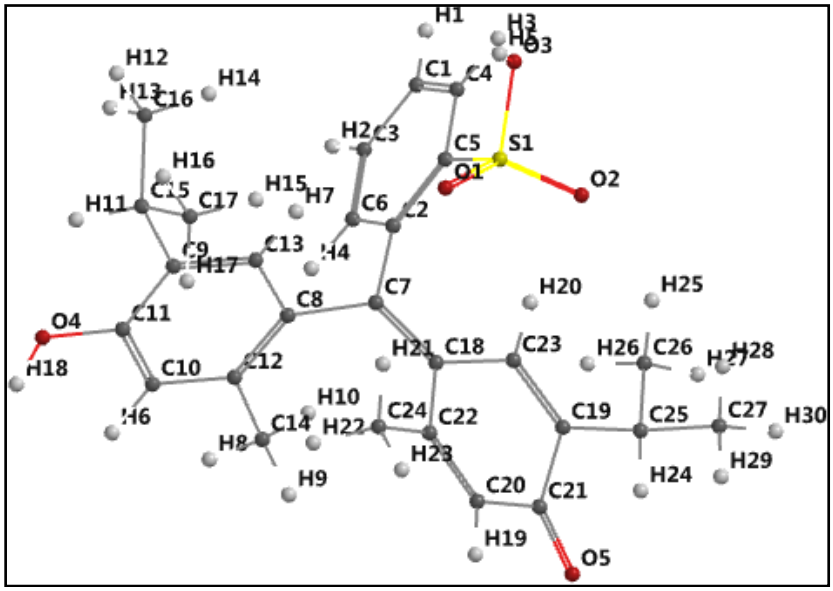


Fig. 2 – Skeletal formula with labeled atoms (Hartree-Fock Method).

Fig. 2 shows the TB skeletal formula. The atoms are labeled to be able to subsequently express the lengths of chemical bonds between the atoms of the molecule as well as the dihedral angles.

2. Simulation Details

The Spartan program provides the access to a number of modern computational methods (molecular mechanics, semi-empirical and Hartree-Fock molecular orbital models) and correlated models including density functional models and Møller-Plesset models. Spartan program offers the access to several spectral quantities, such as infrared spectra, Raman spectra, NMR spectra and UV/visible spectra. Experimental spectra from public online databases may be accessed and overlay onto calculated spectra

Spartan provides graphical tools to improve the interpretation of the results of calculations. Molecular orbitals, electron and spin densities, local ionization potentials and electrostatic potentials can be displayed as surfaces, slices and property maps. Spartan can display some important graphical quantities resulting from quantum chemical calculations: the electron density (shows how much space a molecule occupies), the bond density (reveals chemical bonds) and key molecular orbitals (that provide information about chemical reactivity) (Young, 2001).

The molecular mechanics module calculates the energy, equilibrium geometry and vibrational frequencies. The semi-empirical module calculates the heat of formation, wavefunction, equilibrium and transition-state geometries and vibrational frequencies. The Hartree-Fock module calculates the energy and wave function, equilibrium and transition-state geometries and vibrational frequencies. The density functional module calculates the energy and wave function, equilibrium and transition-state geometries and vibrational frequencies.

Semi-empirical models are the simplest methods based on quantum mechanics. They are applicable to molecules containing 100 - 200 atoms and provide geometries in good accord with experimental structures. Semi-empirical models are suitable for evaluation of properties that depend solely on geometry (such as polar surface area). Semi-empirical models are available for the calculation of IR spectra but do not provide a very good account. They are not available for the calculation of Raman, NMR or UV/visible spectra.

Hartree-Fock models follow from the Schrödinger equation by requiring that the electrons be independent particles (the Hartree-Fock approximation). The motions of electrons in molecules (molecular orbitals) are approximated by a sum of the motions of electrons in atoms (atomic orbitals). Hartree-Fock models are available for the calculation of IR, Raman, NMR and UV/visible spectra. IR (Raman) frequencies are typically overestimated by 10-15% and NMR chemical shifts show large variations from experimental values. Density functional models are to be preferred (Spartan'14 for Windows, 2014).

3. Computational Results

Fig. 3 illustrates the chemical structure of the thymol blue molecule, optimized by Spartan'14 program, using Hartree-Fock method. The arrow indicates the orientation of the dipole moment, a vectorial physical quantity that is a measure of the separation of the electrical charges of a molecule.

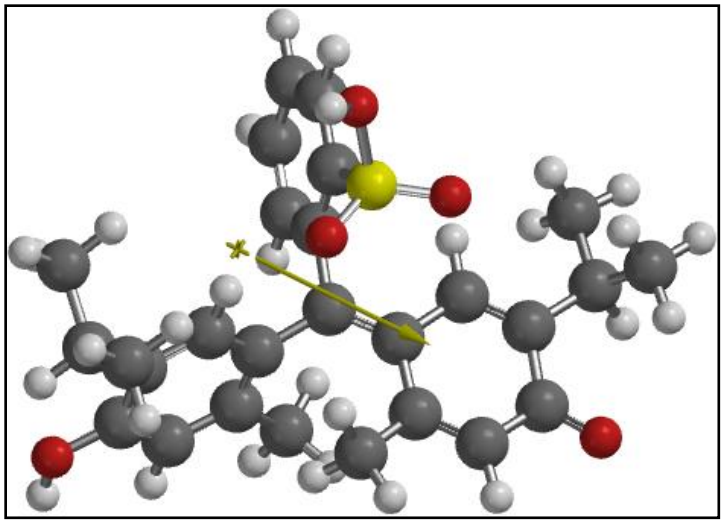


Fig. 3 – Chemical structure of thymol blue, optimized by Spartan'14 program (C – grey, S – yellow, O – red, H – white), Hartree-Fock Method.

The properties of thymol blue molecule were computed using three different methods offered by Spartan program: Hartree-Fock models, semi-empirical models and molecular mechanics models. The molecular parameters obtained in quantum-chemical analysis are listed in Table 1. One can see that the three methods give appropriate values for some information such as weight, number of tautomers, area, volume, polar surface area, ovality, log P, polarizability, hydrogen bond donor count and hydrogen bond acceptor count. The values obtained for energy, energy (aq.), solvation energy, E_{HOMO}, E_{LUMO}, dipole moment and conformers are different.

The charge distribution in a molecule can provide critical insight into its physical and chemical properties. Chemical reactions are also associated with charged sites, and the most highly-charged molecule, or the most highly-charged site in a molecule, is often the most reactive. The sign of the charge is also important. Positively-charged sites in a molecule invite attack by bases and nucleophiles, while negatively-charged sites are usually targeted by acids and electrophiles (http://www.quimica.urv.es/~bo/).

One way to describe a molecule's charge distribution is to give a numerical atomic charge for each atom. A particularly simple and familiar recipe yields so-called formal charges directly from Lewis structures.

Table 1
Molecular Properties of Thymol Blue Molecule, Computed with Spartan'14 Program

Method of Spartan'14	Hartree-Fock Models	Semi-Empirical PM3 Models	Molecular Mechanics Models
Molecule Properties			
Formula	$C_{27}H_{30}O_5S$	$C_{27}H_{30}O_5S$	$C_{27}H_{30}O_5S$
Weight	466.598 amu	466.598 amu	466.598 amu
Energy	-1801.97521 au	-589.36 kJ/mol	201.78 kJ/mol
Energy (aq)	-1802.00114 au	-660.64 kJ/mol	110.14 kJ/mol
Solvation E	-68.08 kJ/mol	-71.28 kJ/mol	-91.64 kJ/mol
E HOMO	-8.11 eV	-9.06 eV	-
E LUMO	1.35 eV	-1.08 eV	-
Dipole Moment	7.88 debye	5.31 debye	6.27 debye
Tautomers	5	5	5
Conformers	384	768	768
Quantitative Structure-Activity Relationship (QSAR)			
Area	476.90 $Å^2$	484.73 $Å^2$	489.68 $Å^2$
Volume	472.19 $Å^3$	475.34 $Å^3$	478.23 $Å^3$
PSA	83.390 $Å^2$	88.354 $Å^2$	86.359 $Å^2$
Ovality	1.63	1.65	1.66
Log P	2.54	2.54	2.54
Polarizability	77.45 $Å^3$	78.05 $Å^3$	-
HBD Count	1	1	1
HBA Count	2	2	2
Temperature	298.15 K	298.15 K	298.15 K

Unfortunately, formal charges are arbitrary. In fact, all methods for assigning charge are arbitrary and necessarily bias the calculated charges in one way or another. This includes methods based on quantum mechanics. Mulliken Charge, Electrostatic Charge and Natural Charge for thymol blue molecule, computed using Hartree-Fock and Semi- Empirical PM3 methods of Spartan program, are displayed in Figs. 4-9. The most used charge partitioning scheme are Mulliken Populations which assign charge to an atomic center on the basis of the total electron density in basis functions located on that center. Natural Population Analysis (NPA) is an algorithm that involves partitioning the charge into atomic orbitals on each center, constructed by dividing the electron density matrix into sub-blocks with the appropriate symmetry. NPA is much less basis set dependent than Mulliken Populations (Leach, 2001; Manz and Gabaldon-Limas, 2016; Reed *et al*., 1985).

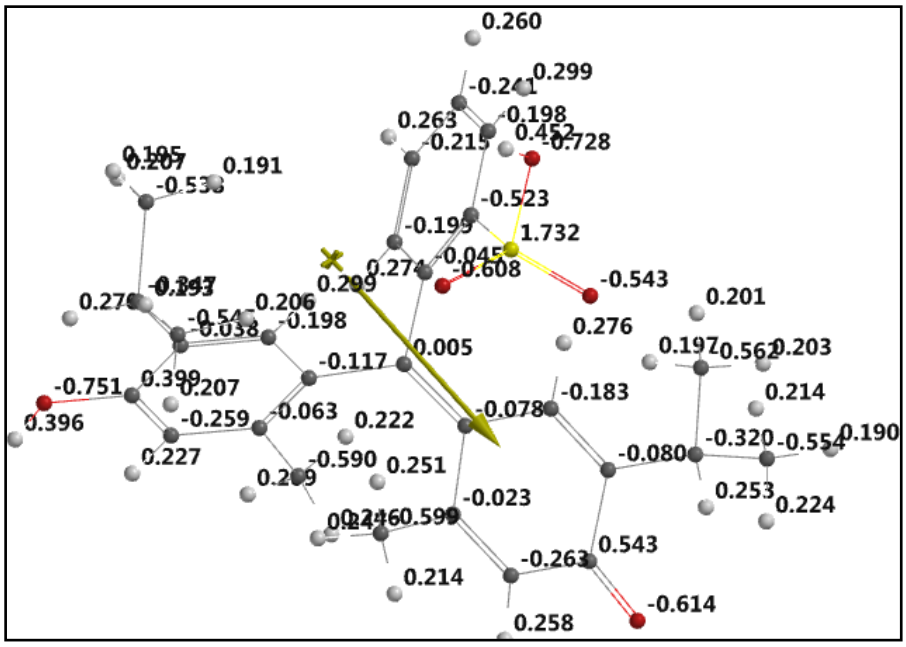


Fig. 4 – Mulliken Charge of molecule, using Hartree-Fock Method of Spartan.

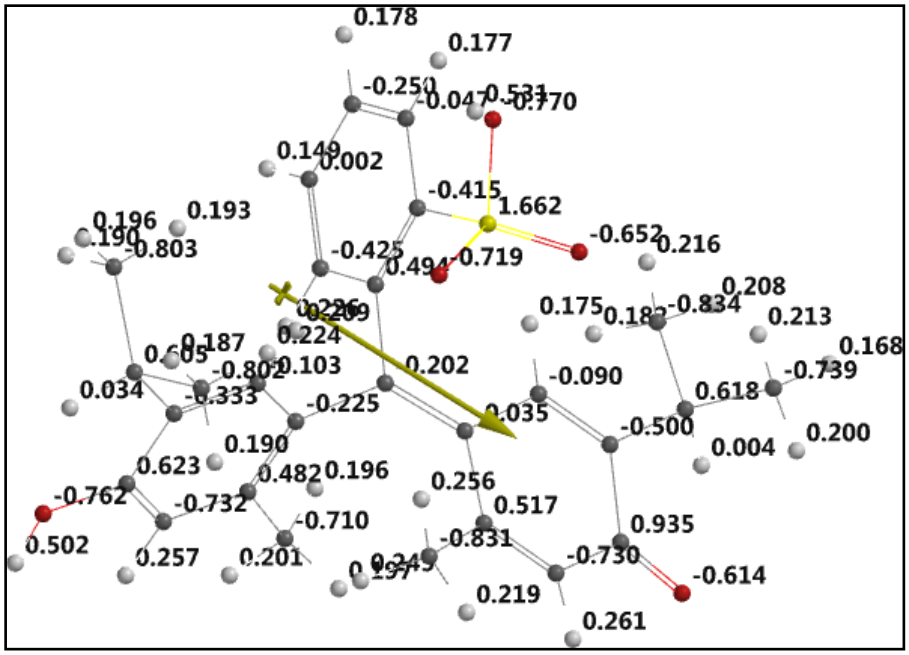


Fig. 5 – Electrostatic Charge of molecule, using Hartree-Fock Method of Spartan.

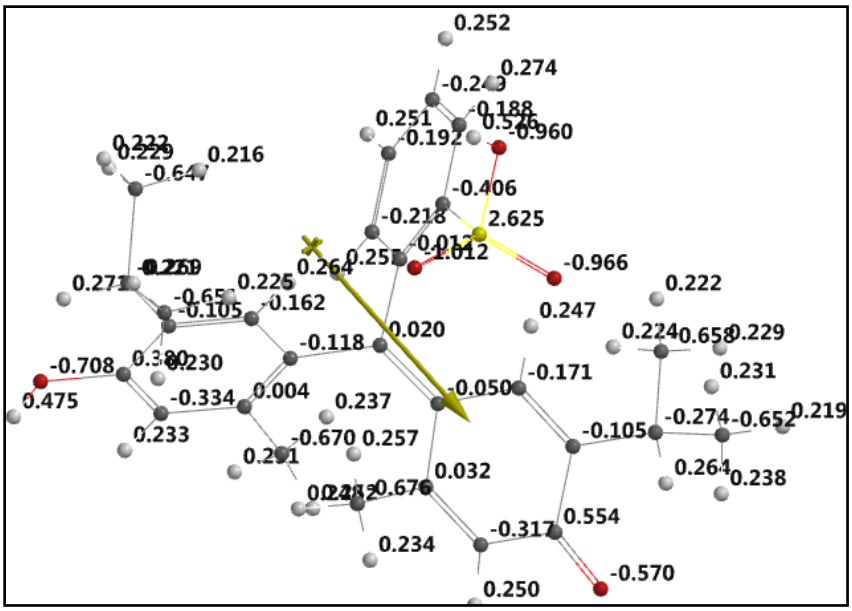


Fig. 6 – Natural Charge of molecule, using Hartree-Fock Method of Spartan.

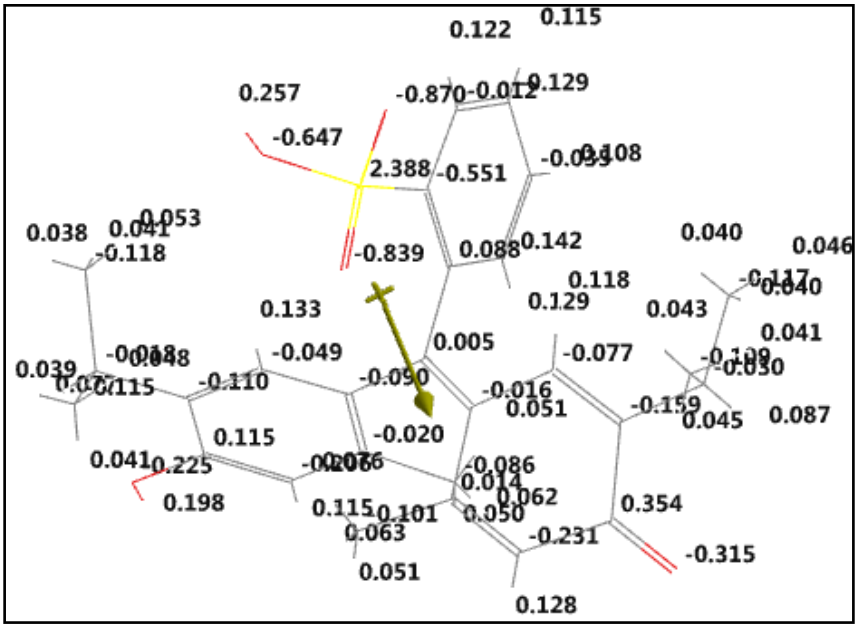


Fig. 7 – Mulliken Charge of thymol blue molecule, using Semi-Empirical PM3 Method of Spartan.

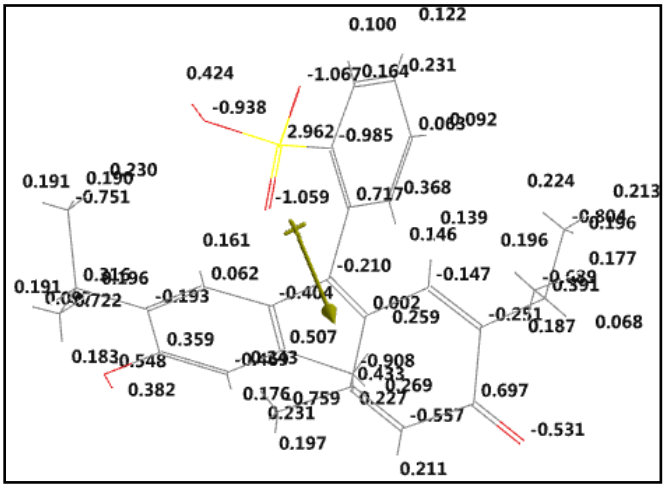


Fig. 8 – Electrostatic Charge of of thymol blue molecule molecule, using Semi-Empirical PM3 Method of Spartan.

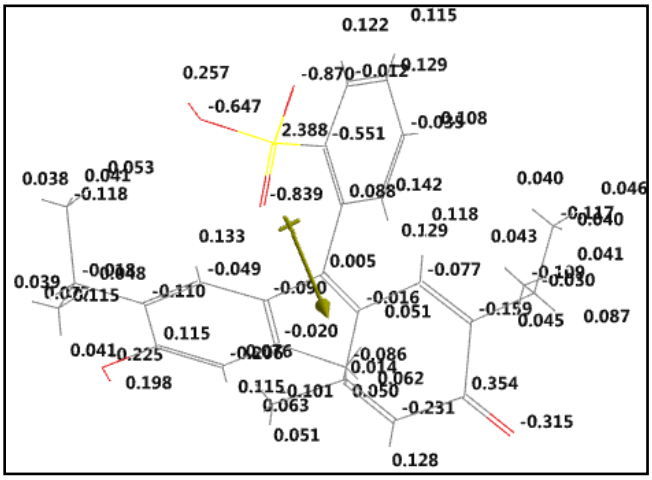


Fig. 9 – Natural Charge of of thymol blue molecule molecule, using Semi-Empirical PM3 Method of Spartan.

The Spartan program can be used to calculate the lengths of chemical bonds between the atoms of the molecule, the angles between these bonds and dihedral angles. The lengths of chemical bonds are listed in Table 2. As can it be seen, the longest chemical bonds are C5-S1 (1.777 Å), S1-O3 (1.616 Å), C25-C26 (1.534 Å), C15-C16, C15-C17, C25-C27 (1.532 Å), while the shortest chemical bonds are O4-H18 (0.971 Å), O3-H5 (0.981 Å), C23-H20 (1.083 Å), C20-H19 (1.084 Å), C10-H6, C13-H7 (1.087 Å), C1-H1, C3-H2, C6-H4 (1.088 Å), C4-H3 (1.089 Å).

Table 2
Lengths of Chemical Bonds of Thymol Blue Molecule, Computed by Hartree-Fock Method of Spartan Program

Chemical bond	Bond length (Å)	Chemical bond	Bond Length (Å)	Chemical bond	Bond Length (Å)	Chemical bond	Bond Length (Å)
C1=C4	1.393	C7-C8	1.503	C15-H11	1.096	C23-H20	1.083
C4-C5	1.406	C8-C13	1.407	C15-C16	1.532	C22-C24	1.506
C5=C2	1.409	C13=C9	1.407	C16-H12	1.096	C24-H21	1.095
C2-C6	1.408	C9-C11	1.396	C16-H13	1.096	C24-H22	1.092
C6=C3	1.397	C11=C10	1.396	C16-H14	1.095	C24-H23	1.097
C3-C1	1.391	C10-C12	1.406	C15-C17	1.532	C20-H19	1.084
C1-H1	1.088	C12=C8	1.413	C17-H15	1.096	C21=O5	1.226
C3-H2	1.088	C13-H7	1.087	C17-H16	1.095	C19-C25	1.519
C6-H4	1.088	C10-H6	1.087	C17-H17	1.096	C25-H24	1.098
C4-H3	1.089	C11-O4	1.367	C7=C18	1.372	C25-C26	1.534
C5-S1	1.777	O4-H18	0.971	C18-C22	1.485	C26-H25	1.096
S1-O3	1.616	C12-C14	1.506	C22=C20	1.345	C26-H26	1.096
S1-O2	1.445	C14-H8	1.096	C20-C21	1.478	C26-H27	1.096
O3-H5	0.981	C14-H9	1.094	C21-C19	1.494	C25-C27	1.532
S1=O1	1.445	C14-H10	1.093	C19=C23	1.346	C27-H28	1.096
`C2-C7	1.503	C9-C15	1.521	C23-C18	1.478	C27-H29	1.095
						C27-H30	1.095

The measure of some dihedral angles is listed in Table 3.

Table 3
The Measure of Some Dihedral Angles for Thymol Blue Molecule, Computed by Hartree-Fock Method of Spartan Program

Dihedral angle	Measure	Dihedral angle	Measure
(C5,C2,C6,C7)	178.77°	(C5,S1,O1,O2)	128.87°
(C6,C2,C7,C8)	63.77°	(C2,C7,C8,C18)	173.63°
(C2,C7,C8,C13)	68.11°	(C2,C7,C18,C22)	169.19°
(C18,C7,C8,C12)	26.60°	(C2,C7, C18,C23)	11.35°
(C7,C8,C12,C10)	178.98°	(C23,C18,C22,C20)	20.39°
(C12,C10,C11,O4)	179.89°	C18,C23,C19,C21)	2.66°
(C13,C9,C11,O4)	0.92°	(C19,C21,C20,C22)	14.53°
(C9,C11,C10,O4)	179.99°	(C18,C22,C20,C24)	173.35°
(C13,C9,C15,C16)	60.77°	(C19,C21,C20,O5)	1.71°
(C9,C15,C16,C17)	124.68°	(C23,C19,C21,C25)	179.06°
(C2,C5,C4,S1)	0.22°	(C23,C19,C25,C26)	9.13°
(C6,C2,C5,S1)	0.33°	(C25,C19,C21,O5)	171.13°
(C5,S1,O1,O3)	111.71°	(C19,C25,C26,C27)	127.23°
(C5,S1,O2,O3)	112.23°	(C21,C19,C25,C27)	78.55°

HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) frontier orbitals (Miller, 2004) for thymol blue molecule are displayed in Fig. 10 (*a*, *b*) and Fig. 11 (*a*, *b*), using Hartree-Fock method of Spartan and Semi-Empirical PM3 method of Spartan, respectively. The energy difference between the HOMO and LUMO is generally the lowest energy electronic excitation that is possible in a molecule. The energy of the HOMO-LUMO gap offers information about what wavelengths are absorbed by the compounds (Holtjie *et al*., 2003).

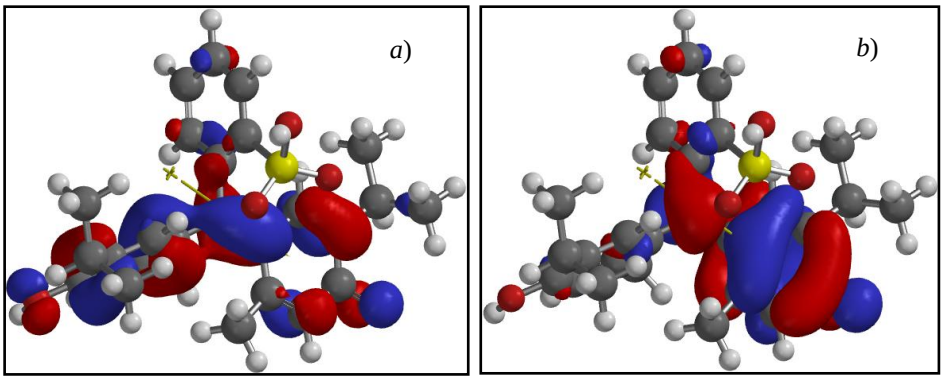


Fig. 10 – HOMO (*a*) and LUMO (*b*) surfaces for thymol blue molecule, obtained with Hartree-Fock method.

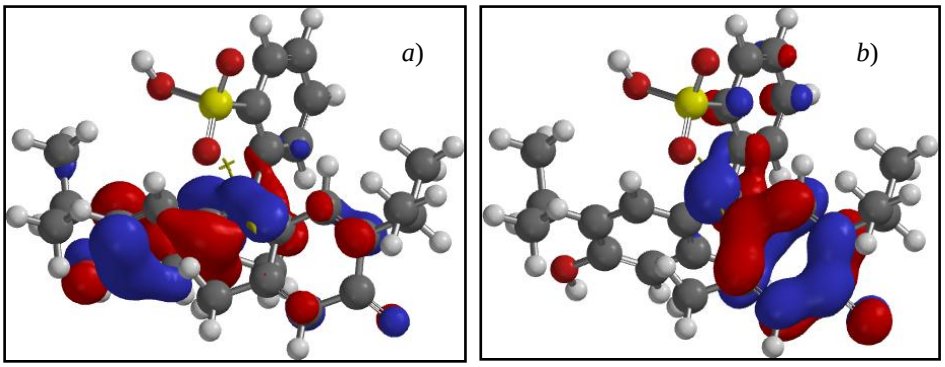


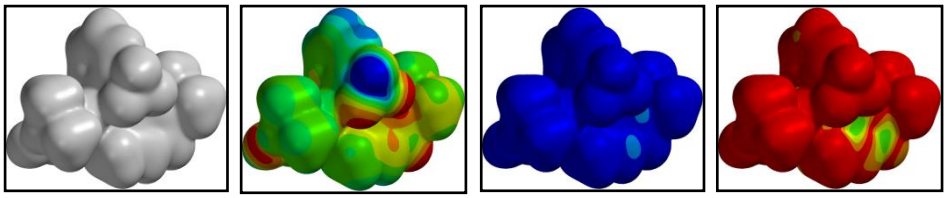
Fig. 11 – HOMO (*a*) and LUMO (*b*) surfaces for thymol blue molecule, obtained with Semi-Empirical PM3 method.

The electron density surface depict overall molecular size and shape of the molecule. Electrostatic potential maps illustrate the space distribution of the electrical charge of a molecule (Shusterman and Shusterman, 1997).

Knowing the distribution of the electrical charge of a molecule, one can determine how the molecule interacts with other molecules (Hehre *et al*., 1998;

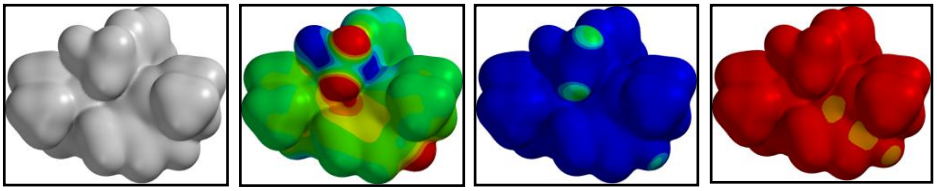
Hehre, 2003). The local ionization potential provides a measure of the relative ease of electron removal ("ionization") at any location around a molecule. In |LUMO| map, the absolute value of the lowest-unoccupied molecular orbital is mapped onto an electron density surface. This offers information about where an electron pair (a nucleophile) might attack. The LUMO map show the regions of a molecule that are are most electron deficient, and therefore, the regions that may be subject to nucleophilic attack (Schlick, 2002).

Density surface, electrostatic potential map, local ionization potential map and |LUMO| map, obtained using the two different methods of Spartan, are displayed in Fig. 12 (*a-d*) and Fig. 13 (*a-d*), respectively.



a) *b*) *c*) *d*)

Fig. 12 – Density surface (*a*), electrostatic potential map (*b*), local ionization potential map (*c*) and |LUMO| map (*d*) with Hartree-Fock method.



a) *b*) *c*) *d*)

Fig. 13 – Density surface (*a*), electrostatic potential map (*b*), local ionization potential map (*c*) and |LUMO| map (*d*) with Semi-Empirical PM3 method.

4. Conclusions

Some differences between the computed molecular parameters using three methods from Spartan 14 are observable, but the order of magnitude and sign of the charges values, of the electron density, electron gap and of the other molecular characteristics is kept in the computational results. The three methods of Spartan show similar more reactive zones of TB molecule both for nucleophilic or electrophylic attack. The sign obtained for logP is the same in all three methods, emphasizing the hydrophilicity of TB.

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CARACTERIZAREA CUANTO-MECANICĂ A TIMOLULUI BLUE

(Rezumat)

Timol blue (TB) este un important indicator acido-bazic de culoare utilizat în diverse aplicații. Parametrii acestuia în starea fundamentală sunt foarte importanți, așa încât am realizat un studiu comparativ al parametrilor fizici ai TB cu trei metode diferite din programele Spartan 14, în vederea stabilirii celei mai bune metode pentru a fi utilizată în viitoarele noastre aplicații spectrale.

După optimizarea geometrică, principalii parametri ai TB, cum sunt lungimea legăturilor chimice, sarcinile electrice din vecinătatea atomilor componenți, unghiurile diedre, momentul de dipol și polarizabilitatea moleculară, au fost calculați.