Quantum Genetics and Quantum Automata Models of Quantum-Molecular Evolution Involved in the Evolution of Organisms and Species

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I.C. Baianu

AFC-NMR & NIR Microspectroscopy Facility,
College of ACES, FSHN & NPRE Departments,
University of Illinois at Urbana,
Urbana, IL. 61801, USA
Email address: **ibaianu @illinois.edu**

1. Introduction

Previous theoretical or general approaches (Rosen, 1960; Shcherbik and Buchatsky, 2007) to the problems of Quantum Genetics and Molecular Evolution are considered in this article from the point of view of Quantum Automata Theory first published by the author in 1971 (Baianu,1971a, b) , and further developed in several recent articles (Baianu, 1977, 1983, 1987, 2004, 2011).

It is often assumed incorrectly that Quantum Computation was introduced in 1982 by Richard Feynman and also that Quantum Automata were introduced in 1997. Actually, the formal concepts of Quantum Automata and Quantum Computation were introduced in the (Baianu, 1971a), in relation to Quantum Genetics (Rosen, 1960). There are also numerous citations of Quantum Automata papers printed in the late 80's and also recent quantum computation textbooks that fail to report the first formal introduction of the concepts of *quantum automaton* and *quantum computation*. Categorical computations, both algebraic and topological, were also introduced in 1971 (Baianu, 1971b) that proposed to employ symbolic programming for adjoint functor pairs in the theory of categories, functors and natural transformations (Baianu, 1971b). The notions of topological semigroup, quantum automaton and quantum computer, were then suggested for applications and modeling, with a view to their potential applications to the analogous simulation of biological systems, and especially genetic activities and nonlinear dynamics in genetic networks. Further, detailed studies of nonlinear dynamics in genetic networks were carried out in categories of n-valued, Łukasiewicz Logic Algebras that showed significant dissimilarities (Baianu, 1977) from Boolean models of human neural networks (McCullough and Pitts, 1943). Further, detailed studies of nonlinear dynamics in genetic networks were carried out in categories of *n*-valued, Łukasiewicz Logic Algebras (Baianu, 1977; 2004a; Baianu et al, 2004b) that showed most significant dissimilarities from Boolean models of human neural networks

(McCullough and Pitts, 1943). The concepts of quantum automata and quantum computation were thus studied in the context of quantum genetics and genetic networks with nonlinear dynamics (Baianu, 1977, 1987), and the results and predictions of the new theory of quantum genetic networks were then compared with those of random or cyclic Boolean models of genetic networks that abound in the literature. It turns out the any Bayesian, or Boolean, model of the genomes-- including the human genome—exhibit quite different behaviors from that of the actual quantum genomes (Baianu, 1987, 2004, 2011). Thus, classical automata theory has only very limited relevance to modeling of genomes and interactomes.

2. Genome Represented as Quantum Automata

In previous publications (Baianu,1971a,b) the formal concept of quantum automaton and quantum computation, respectively, were introduced and their possible implications for genetic processes and metabolic activities in living cells and organisms were considered. This was followed by a report on quantum and abstract, symbolic computation based on the theory of categories, functors and natural transformations (Baianu, 1971b; 1977; 1987; 2004; Baianu et al, 2004). The notions of topological semigroup, quantum automaton, or quantum computer, were then suggested with a view to their potential applications to the analogous simulation of biological systems, and especially genetic activities and nonlinear dynamics in genetic networks.
Such theoretical developments make a significant impact also on improving our understanding of both molecular and biological evolution that was first attempted, *without success*, in terms of the older quantum mechanics theories by Erwin Schrödinger (1944), and subsequently by Robert Rosen (1960) in terms of an application of the early quantum theory of Von Neumann.

Further, detailed studies of nonlinear dynamics in genetic networks were later carried out in categories of n-valued, Łukasiewicz logic algebras (**LM$_n$**) that showed significant dissimilarities (Baianu, 1977; 2004a; Baianu et al, 2004b) from Boolean models of human neural networks (McCullough and Pitts, 1943); the results obtained with such **LM$_n$** logic algebras follow naturally from a formal development of quantum logic in terms of non-Abelian, non-distributive many-valued logics. Molecular models in terms of categories, functors and natural transformations were then formulated for uni-molecular chemical transformations, multi-molecular chemical and biochemical transformations (Baianu, 1983, 1987, 2004a). Previous applications of computer modeling, classical automata theory, and relational biology to molecular biology, oncogenesis and medicine were extensively reviewed and several important conclusions were reached regarding both the potential and limitations of the computation-assisted modeling of biological systems, and especially complex organisms such as Homo sapiens sapiens (Baianu,1987). Novel approaches to solving the realization problems of Relational Biology models in Complex System Biology are

introduced in terms of natural transformations between functors of such molecular categories. Several applications of such natural transformations of functors were then presented to protein biosynthesis, embryogenesis and nuclear transplant experiments. Topoi of Łukasiewicz Logic Algebras and Intuitionistic Logic (Heyting) Algebras are being considered for modeling nonlinear dynamics and cognitive processes in complex neural networks that are present in the human brain, as well as stochastic modeling of genetic networks in Łukasiewicz Logic Algebras.

3. Quantum Automata and Quantum Dynamics in terms of the Theory of Categories, Functors and Natural Transformations

Molecular models in terms of categories, functors and natural transformations were then formulated for uni-molecular chemical transformations, multi-molecular chemical and biochemical transformations (Baianu, 1983, 2004a). Previous applications of computer modeling, classical automata theory, and relational biology to molecular biology, oncogenesis and medicine were extensively reviewed and several important conclusions were reached regarding both the potential and limitations of the computation-assisted modeling of biological systems, and especially complex organisms such as *Homo sapiens sapiens* (Baianu,1987).

3.1. Quantum Genetics and Molecular Models in terms of LM_n Logics, Categories and Natural Transformations

Previous classical models of molecular transformations in terms of molecular sets can be rephrased in terms of modern quantum operator algebra and Category Theory. Consider the simple case of uni-molecular reactions that will be then extended to multi-molecular, chemical and biochemical, reactions:

$$T : A \times I \rightarrow B \times I \quad,$$

where **A** is the original sample set of molecules, **I** = **[***0, t***]** is a finite segment of the real time axis and **A x I** denotes the indexing of each **A**-type molecule by the instant of time at which each molecule *a* ε *A* is actually transforming into a *B*-type molecule. **B x I** denotes the set of the newly formed **B**-type molecules which are indexed by their corresponding instants of birth.

MOLECULAR SET -**A**, with f: A → A are ENDOMORPHISMS
that belong to H(A,A)

THE CATEGORY OF MOLECULAR SETS AND THEIR TRANSFORMATIONS
 is **M** .

THE h^X FUNCTOR: h^A: **M** → **Set**   is defined as:

   $h^A(X}$ = H(A,X) for any X in **M**
   h^A (t) = m: H(A,A) → H(A,B) for any t: A→B, where:

   A = MOLECULAR SET
   B= MOLECULAR SET OF REACTION PRODUCTS OF TYPE "B",
   resulting from a definition of the molecular set variable (m.s.v.), defined as
   follows:

The flexible notion of molecular set variable (m.s.v) is precisely represented by the morphisms **v**
in the following diagram:
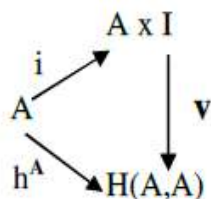
where morphisms **v** are induced by the inclusion mappings *i*: A→A x I and the commutativity
conditions h^A = v o *i* . The naturality of this diagram simply means that such conditions hold for
any functor h^A defined as above.

THE REPRESENTATION OF UNIMOLECULAR CHEMICAL REACTIONS AS **NATURAL TRANSFORMATIONS**:

The unimolecular chemical reaction can be thus represented by the <u>natural</u> transformations $h^A \xrightarrow{\quad \eta \quad} h^B$, as one can readily check in the commutative diagram :

$$
\begin{array}{ccc}
h^A(A) = H(A,A) & \xdashrightarrow{\quad \eta_A \quad} & h^B(A) = H(B,A) \\[2em]
\Big\downarrow h^A(t) & & \Big\downarrow h^B(t) \\[2em]
h^A(B) = H(A,B) & \xdashrightarrow{\quad \eta_B \quad} & h^B(B) = H(B,B)
\end{array}
$$

if the states of the molecular sets $A_u = a_1, \ldots, a_n$ and $B_u = b_1, \ldots b_n$ are represented by certain endomorphisms in $H(A,A)$ and $H(B,B)$, respectively.

The <u>OBSERVABLE</u> of an <u>m.s.v</u>, <u>B,</u> characterizing the chemical products "B" of a **chemical reaction** is a <u>MORPHISM</u>:

$$\gamma : H\underline{(B,B)} \dashrightarrow R$$

where R is the set of real numbers .

THIS OBSERVABLE IS SUBJECT TO THE FOLLOWING COMMUTATIVITY or NATURALITY CONDITION:

$$
\begin{array}{ccc}
H(A,A) & \xdashrightarrow{\quad c \quad} & H(B,B) \\
& & \\
\alpha \searrow & & \swarrow \gamma^{\kappa} \\
& R &
\end{array}
\qquad (5)
$$

with $c : A_u^* \longrightarrow B_u^*$,   and A*, B* being specially prepared **fields of states**, within a measurement uncertainty range, <u>δ.</u>
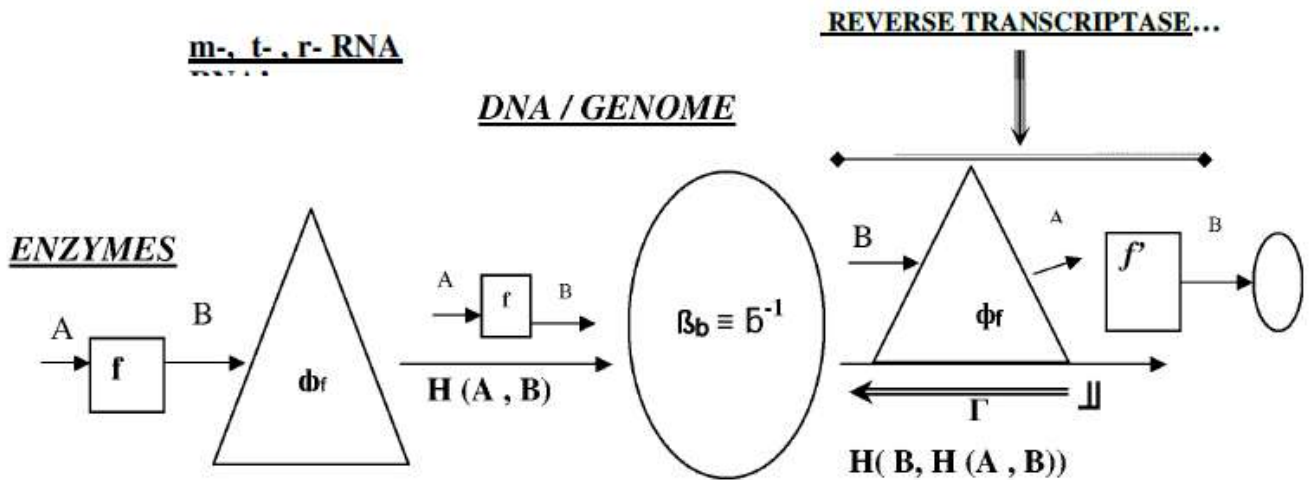
DEFINITION OF A *MULTI-MOLECULAR REACTION* :

In the case of *multi-molecular reactions*, the canonical functor of category theory:

h : $\underline{M}$ −·−·−·−▶ [M, Set]   (4)

assigns to each molecular set $\underline{A}$ the functor $h^{A\cdot}$ and to each chemical transformation

t: A ⟶ B, the natural transformation $h^A \xrightarrow{\eta} h^B$.

The simplest METABOLIC-REPAIR (M, R)-System with REVERSE TRANSCRIPTION.

DNA DUPLICATION and CELL DIVISION follows next in this series-type, or **linear** categorical diagram.

Figure 1. A representation of DNA duplication and cell division in terms of quantum automata and *generalized (M,R)-system with quantum observables* in categorical diagrams of molecular variable classes.

Possible molecular candidates are indicated at the top of the diagram in **Figure 1**, above the corresponding METABOLIC (f) or REPAIR/ TRANSCRIPTION (ϕ_f) components. Surviving organisms have **non-linear** diagrams *with* **feedback** and **feedforward**. note in this case, the '**closure', functional mapping, г,** that physically regenerates the telomere and closes the dna-loop at the end of the chromosome. (note also that the above diagram in fig.1 was updated in 2004; the original diagram in 1983 was **completely linear**, and did not have the **closure map г**, the telomere, the **reverse transcriptase... and the dna duplication** *that are now all represented in the updated diagram. Adding to this diagram an* hTERT *suppressor gene would provide a* **FEEDBACK** *mechanism for simulating the control of cell division and the possibility of cell cycle arrest* **only in somatic cells**. **The addition of an** *hTERT promoter gen*, is however the preferred

alternative because such a gene could be activated to induce 'perpetual cell cycling through the cell divison, as in the so-called `*immortal cell lines'.* This representation also affords the consideration of simple models of *carcinogenesis and malignant tumors*.

4. Conclusions

The representation of genomes and Interactome networks in categories of many-valued logic *LMn –*algebras that are naturally transformed during biological evolution, or evolve through interactions with the environment provide a new insight into the mechanisms of *molecular evolution,* as well as *organismal evolution*, in terms of sequences of quantum automata. Phenotypic changes are expressed *only* when certain environmentally-induced quantum-molecular changes are coupled with an *internal* re-structuring of major submodules of the genome and Interactome networks related to cell cycling and cell growth. Contrary to the commonly held view of `standard' Darwinist models of evolution, the evolution of organisms and species occurs through coupled multi-molecular transformations induced not only by the environment but actually realized through internal re-organizations of genome and interactome networks. The biological, evolutionary processes involve certain epigenetic transformations that are responsible for phenotypic expression of the genome and Interactome transformations initiated at the quantum-molecular level. It can thus be said that only quantum genetics can provide correct explanations of evolutionary processes that are initiated at the quantum--multi-molecular levels and propagate to the higher levels of organismal and species evolution.

Biological evolution should be therefore regarded as a *multi-scale* process which is initiated by underlying *quantum (coupled) multi-molecular transformations* of the genomic and interactomic networks, followed by specific phenotypic transformations at the level of organism and the *variable* biogroupoids associated with the evolution of species which are essential to the survival of the species. The theoretical framework introduced in this article also paves the way to a Quantitative Biology approach to biological evolution at the quantum-molecular, as well as at the organismal and species levels. This is quite a substantial modification of the `established' modern Darwinist, and also of several so-called `molecular evolution' theories.

Cited References

Baianu, I.1971a. "Organismic Supercategories and Qualitative Dynamics of Systems**."** *Bull. Math. Biophys***., 33**: 339-353**.**

Baianu, I. 1971. Categories, Functors and Automata Theory**.** *The 4th Intl. Congress LMPS, Proceedings,* August-Sept. 1971b.

Baianu, I. and Scripcariu, D. 1973. On Adjoint Dynamical Systems. *Bull. Math. Biology*, **35**: 475-486.

Baianu, I. 1973. Some Algebraic Properties of (M,R)-Systems in Categories. *Bull. Math. Biophys.,* **35:** 213-218.

Baianu, I. and Marinescu, M. 1974. A Functorial Construction of (M,R)-Systems**.** *Rev. Roum. Math. Pures et Appl***., 19:** 389-392**.**

Baianu, I.C. 1977. A Logical Model of Genetic Activities in Lukasiewicz Algebras: The Non-Linear Theory., *Bull. Math. Biol*.,**39**:249-258.

Baianu, I.C. 1980. Natural Transformations of Organismic Structures. Bull.Math. Biology, **42**:431-446.

Baianu, I.C.1983. Natural Transformations Models in Molecular Biology. *SIAM Natl. Meeting*, Denver, CO, USA.

Baianu, I.C. 1984. A Molecular-Set-Variable Model of Structural and Regulatory Activities in Metabolic and Genetic Systems., *Fed. Proc. Amer. Soc. Experim. Biol*. **43**:917.

Baianu, I.C. 1987. "Computer Models and Automata Theory in Biology and Medicine" (A Review). In: "*Mathematical models in Medicine*.",vol.7., M. Witten, Ed., Pergamon Press: New York, pp.1513-1577.

Baianu, I.C. 2004. "Cell Genome and Interactome Nonlinear Dynamic Models in Łukasiewicz Logic Algebras. Neoplastic Transformation Models in a Łukasiewicz Topos." *Cogprints preprint*, June 25th, 2004. # GN 0406050.

Baianu, I.C., J. Glazebrook, G. Georgescu and R.Brown, 2006. "A Novel Approach to Complex Systems Biology and Observation Strategies based on Categories, Higher Dimensional Algebra and Łukasiewicz Topos. " *Axiomathes*, 16 pp.

Carnap. R. 1938. "*'The Logical Syntax of Language*" New York: Harcourt, Brace and Co.

Georgescu, G. and C. Vraciu 1970. "On the Characterization of Lukasiewicz Algebras." *J. Algebra*, **16** (4): 486-495.

Hilbert, D. and W. Ackerman. 1927. *Grunduge der Theoretischen Logik*, Berlin: Springer.

Levine, Raphael D. (2005). *Molecular Reaction Dynamics*. Cambridge University Press. ISBN 978-0521842761.

McCulloch, W and W. Pitts. 1943. "A Logical Calculus of Ideas Immanent in Nervous Activity" *Bull. Math. Biophys.*, **5**: 115-133.

Rosen, R.1958.a."A Relational Theory of Biological Systems" Bull. Math. Biophys., 20, 245-260.

Rosen, R. 1958b. "The Representation of Biological Systems from the Standpoint of the Theory of Categories" *Bull. Math. Biophys.*, 20: 317-341.

Rosen, R. 1960. "A quantum-theoretic approach to genetic problems." *Bulletin of Mathematical Biophysics*, **22**: 227-255.

Robert Rosen. 1970. *Dynamical Systems Theory in Biology*, New York: Wiley Interscience.

Rosen, Robert. 1973. "On the Dynamical realization of (M,R)-Systems." Bull. Math. Biology., **35**: 1-10.

Rosen, Robert. 2001. "*Essays on Life Itself* ". New York: Columbia University Press, 221 pp.

Russel, Bertrand and A.N. Whitehead, 1925. *Principia Mathematica*, Cambridge: Cambridge Univ. Press.

Erwin Schrödinger. 1944. *What is Life?* Cambridge, U.K.

Sergi, Alessandro. 2009. "Quantum Biology". *AAPP Physical, Mathematical, and Natural Sciences* **87** (1): no. C1C0901001. doi:10.1478/C1C0901001. ISSN 1825-1242.

Shcherbik, V. V. & Buchatsky, L.P. 2007. *Quantum Genetics.* Enfield, NH : Science Publishers, pp.156*.*

Scholes , G.S. 2010. "Quantum-Coherent Electronic Energy Transfer: Did Nature Think of It First ?" *Journal of Physical Chemistry Letters* **1**: 2–8. doi:10.1021/jz900062f

Warner, M. 1982. Representations of (M,R)-Systems by Categories of Automata., *Bull. Math. Biol*., **44**:661-668.

Quantum Biology. University of Illinois at Urbana-Champaign, Theoretical and Computational Biophysics Group. http://www.ks.uiuc.edu/Research/quantum_biology/

Science Daily *Quantum Biology: Powerful Computer Models Reveal Key Biological Mechanism,* Retrieved Oct 14, 2007, http://www.sciencedaily.com/releases/2007/01/070116133617.htm

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