

ADVANCES IN MATHEMATICS RESEARCH

22
VOLUME

Albert R. Baswell
Editor

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Advances in Mathematics Research



Baswell



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MATHEMATICS RESEARCH**

VOLUME 22

ALBERT R. BASWELL
EDITOR



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VOLUME 22

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PREFACE

“Advances in Mathematics Research” presents original studies on the leading edge of mathematics. Each article has been carefully selected in an attempt to present substantial research results across a broad spectrum. Chapter One summarizes the phase/current generalized measures of the entropy/information content in complex quantum states of molecular systems. Chapter Two reviews the current knowledge regarding Mavridis’ area (MA), with emphasis on the role of applied mathematics in its discovery, as well as to explore its mathematical expression. In Chapter Three a model of fractional difference has been defined by the author as a fractional Newton binomial with respect to the finite difference operator as parameter, therefore they obtained an alternative to fractional derivative, and further, as a by-product, they came across the so-called modified Riemann-Liouville derivative which ascribes a special role to the initial value of the considered function. Chapter Four presents some popular uses of exponential distribution in the context of ordered random variables. Chapter Five gives a comprehensive introduction to the Ricci flow on manifolds of dimension two which can be done in a reasonable fashion when the Euler characteristic is negative or zero. Chapter Six investigates some geometric properties by using the concepts of the geometric function theory and studies the convexity and star-like for the new operator.

Chapter 1 – The phase/current generalized measures of the entropy/information content in complex quantum states of molecular systems are summarized and the *phase*-equilibria are introduced. The equilibrium states represent the *phase*-transformed solutions of the Schrödinger equation. These “thermodynamic” equilibria result from the information-theoretic principle of the maximum resultant entropy combining the classical

(probability) and nonclassical (phase/current) contributions. The entropy continuity problem is addressed using a standard description of the classical irreversible thermodynamics, and local entropy production is shown to be positive in molecular equilibria. These extremum entropy states are also shown to generate the ordinary Fick's migration component in the quantum *probability*-continuity relation interpreted as a "*diffusion*" equation. A finite electronic current generates a mixture of the "*convection*" and "*reaction*" terms in the associated probability-balance equation.

The quantum-mechanical *entanglement* of molecular fragments is approached within both the wavefunction and density-functional theories. The Schrödinger *natural* (*intra*-fragment decoupled) representation of the effective density operators of the complementary molecular fragments in the specified molecular state is addressed and holistic phenomena in such subsystems are explored. The "external" (*inter*-fragment) electron correlation energy is expressed in terms of the relevant (coupling-constant)-averaged hole and the equilibrium analogs of the entangled states of subsystems are discussed. In the Harriman-Zumbach-Maschke construction, of the subsystem wavefunction yielding the specified density, the electron distributions of molecular fragments determine moduli of the state occupied equidensity orbitals, while "thermodynamic" phases of the mutually-*closed* (nonbonded, disentangled) or mutually-*open* (bonded, entangled) subsystems are generated by the fragment and molecular probability distributions, respectively. As an illustration typical hypothetical stages of a chemical reaction in the bimolecular reactive systems $R = A \cdots B$ composed of the Acidic (A) and Basic (B) reactants are examined.

Chapter 2 – Applied mathematics is a broad subject area in the mathematical sciences dealing with those topics, problems and techniques that have been useful in analyzing real-world phenomena. Application of mathematics to several sciences, including medicine, has revolutionarily changed human lives during the last century. Neurosurgery, especially the subspecialty of stereotactic and functional neurosurgery, is certainly one of the medical specialties which have made particular progress due to applied mathematics. Among the currently used stereotactic neurosurgical interventions, deep brain stimulation (DBS), a stereotactic procedure of implantation of thin electrodes into deep brain structures, has a fundamental role. The nucleus accumbens (NA) is the most important pleasure center of the brain and constitutes a modern DBS target for selected patients suffering from severe neuropsychiatric disorders. Stereotactic anatomy of the brain, necessary for applying stereotactic neurosurgical procedures, deals with precise identification and localization of brain structures and distances in stereotactic

space, using a three-dimensional coordinate system. Mavridis' area (MA), the most reliable stereotactically standard part of the human NA, was recently discovered as a result of the application of mathematics to stereotactic anatomy data. It is primarily useful as a guide for NA DBS. The purpose of this chapter is to review the current knowledge regarding MA, with emphasis on the role of applied mathematics in its discovery, as well as to explore its mathematical expression. An innovative idea which was evaluated by some modern studies of stereotactic anatomy was the potential existence of stereotactically standard areas within brain nuclei, i.e., areas resisting to the individual variability of the nuclear location in stereotactic space. In this context, mathematical analysis was applied to the NA stereotactic coordinates (measured on anatomic specimens and magnetic resonance images). This detailed analysis of carefully combined gross anatomic and magnetic resonance imaging data included primarily methods of analytic geometry. The findings confirmed the initial idea and, among the results of this research, stereotactically standard NA areas, definable by specific coordinates, were discovered in 2010. The most powerful and important among them was MA which represents the most reliable stereotactically standard area of the human NA. In Cartesian three-space it is mathematically expressed by the formula $S_M = \{(x,y,z) \in \mathbb{R}^3 : |x| \in [6,9] \wedge y = -2 \wedge z \in [-2,-0.8]\}$. Its unique characteristic is its resistance to the individual variability of the NA location in stereotactic space, remaining unaffected by gender (male-female) and side (right-left). Consequently, MA is expected to be applicable in every adult human brain and is currently the most accurate stereotactic microanatomic guide for targeting the NA. A DBS electrode placed within MA is therefore expected to be absolutely localized within the NA. The example of MA shows how mathematics applied to anatomy, in the context of a carefully designed clinically-oriented study, can offer remarkable results. Under such circumstances mathematical accuracy can be safely translated into microsurgical accuracy; and this is particularly crucial when dealing with minimally invasive interventions within the human brain.

Chapter 3 – A model of fractional difference has been defined by the author as a fractional Newton binomial with respect to the finite difference operator as parameter, therefore we obtained an alternative to fractional derivative, and further, as a by-product, we came across the so-called modified Riemann-Liouville derivative which ascribes a special role to the initial value of the considered function. The key feature of this approach is that the fractional calculus so obtained is not commutative, what is quite consistent with quantum physics on the one hand, and furthermore results in non-

commutative derivative chain rules on the other hand. In this paper, further results are displayed on the applications of this model to various topics. More especially, one considers the relation of this approach with fractional Z-transform and modified Z-transform, the solutions of some fractional differential equations which are nowhere differentiable, and a new approach to fractional Brownian motion with Gaussian white noise as basic generating processes. This fractional calculus seems to be more especially relevant for the study of self-similar functions and non-differentiable functions. One takes this opportunity to come back again on the Leibniz derivative chain rule which is re-named local Leibniz derivative chain rule. This fractional calculus is a non-commutative calculus.

Chapter 4 – Exponential distribution has found widespread applications in ordered random variables. The distribution has been studied by several authors in the context of ordered random variables. This chapter will present some popular uses of exponential distribution in the context of ordered random variables. Recurrence relations for moments of ordered random variables; including *Order Statistics*, *Record Values* and *Generalized Order Statistics*; will be presented. The characterization of distribution of ordered random variables in the context of exponential distribution is also presented. Estimation of parameters of the distribution using ordered data will also be discussed. The authors have also discussed the use of exponential distribution in the context of concomitants of ordered random variables.

Chapter 5 – The study of differentiable manifolds is a deep and extensive area of mathematics. A technique such as the study of the Ricci flow turns out to be a very useful tool in this regard. This flow is an evolution of a Riemannian metric driven by a parabolic type of partial differential equation. It has attracted great interest recently due to its important achievements in geometry such as Perelman’s proof of the geometrization conjecture and Brendle-Schoen’s proof of the differentiable sphere theorem. It is the purpose here to give a comprehensive introduction to the Ricci flow on manifolds of dimension two which can be done in a reasonable fashion when the Euler characteristic is negative or zero. A brief introduction will be given to the case in which the Euler characteristic is positive.

Chapter 6 – In this chapter, the authors construct a new fuzzy space of normalized analytic functions in the open unit disk. This construction takes place on the upper and lower values of the analytic functions in the open unit disk. Moreover, they formulate a new shift-plus differential operator. This operator includes in some classes of the fuzzy normalized analytic function. The authors show that the operator has an upper bound in some Hardy spaces.

They investigate some geometric properties by using the concepts of the geometric function theory. The authors study the convexity and star-like for the new operator. Their method is the Jack Lemma for the minimal and maximal values of the analytic function. The authors illustrate some other discussions describing the topology of the operator.

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Chapter 1

ENTROPY CONTINUITY, ELECTRON DIFFUSION AND FRAGMENT ENTANGLEMENT IN EQUILIBRIUM STATES*

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ABSTRACT

The phase/current generalized measures of the entropy/information content in complex quantum states of molecular systems are summarized and the *phase*-equilibria are introduced. The equilibrium states represent the *phase*-transformed solutions of the Schrödinger equation. These “thermodynamic” equilibria result from the information-theoretic principle of the maximum resultant entropy combining the classical (probability) and nonclassical (phase/current) contributions. The entropy continuity problem is addressed using a standard description of the classical irreversible thermodynamics, and local entropy production is shown to be positive in molecular equilibria. These extremum entropy states are also shown to generate the ordinary Fick’s migration component in the quantum *probability*-continuity relation interpreted as a “*diffusion*” equation. A finite electronic current generates a mixture of the “*convection*” and “*reaction*” terms in the associated probability-balance equation.

The quantum-mechanical *entanglement* of molecular fragments is approached within both the wavefunction and density-functional theories.

The Schrödinger *natural* (*intra*-fragment decoupled) representation of the effective density operators of the complementary molecular fragments in the specified molecular state is addressed and holistic phenomena in such subsystems are explored. The “external” (*inter*-fragment) electron correlation energy is expressed in terms of the relevant (coupling-constant)-averaged hole and the equilibrium analogs of the entangled states of subsystems are discussed. In the Harriman-Zumbach-Maschke construction, of the subsystem wavefunction yielding the specified density, the electron distributions of molecular fragments determine moduli of the state occupied equidensity orbitals, while “thermodynamic” phases of the mutually-*closed* (nonbonded, disentangled) or mutually-*open* (bonded, entangled) subsystems are generated by the fragment and molecular probability distributions, respectively. As an illustration typical hypothetical stages of a chemical reaction in the bimolecular reactive systems $R = A \cdots B$ composed of the Acidic (A) and Basic (B) reactants are examined.

1. INTRODUCTION

The electronic wavefunctions determining quantum states in molecules are complex entities characterized by their *modulus* and *phase* components: the square of the former generates the state particle probability distribution, while the gradient of the latter accounts for its current density. Besides the familiar *stationary* states in quantum mechanics (QM), which exhibit a purely *time*-dependent phase determined by an eigenvalue of the electronic Hamiltonian, and general solutions of the Schrödinger equation (SE), in chemical interpretations of molecular electronic structure and reactive processes of interest also are the *phase*-transformed states originating from entropic principles of Quantum Information Theory (QIT) [1-7]. These *equilibrium* (“thermodynamic”) states correspond to the maximum of the state *resultant* entropy combining the classical (probability) and nonclassical (phase/current) information contributions. Such generalized entropic concepts allow one to distinguish the information content of states generating the same electron density but differing in their current composition.

In entropic theories of molecular electronic structure, e.g., [7-10], one thus requires *quantum* generalizations of the familiar Fisher [11] and Shannon [12]

*The following tensor notation is adopted: A denotes a *scalar*, \mathbf{A} is a row/column *vector*, \mathbf{A} represents a square or rectangular *matrix*, and the dashed symbol \hat{A} stands for the quantum-mechanical *operator* of the physical property A .