QUANTUM NANOSYSTEMS

STRUCTURE, PROPERTIES, AND INTERACTIONS

Editor Mihai V. Putz, PhD





QUANTUM NANOSYSTEMS

Structure, Properties, and Interactions

This page intentionally left blank

QUANTUM NANOSYSTEMS Structure, Properties, and Interactions

Edited by Mihai V. Putz, PhD



CRC Press Taylor & Francis Group 6000 Broken Sound Parkway NW, Suite 300 Boca Raton, FL 33487-2742 Apple Academic Press, Inc 3333 Mistwell Crescent Oakville, ON L6L 0A2 Canada

© 2015 by Apple Academic Press, Inc. Exclusive worldwide distribution by CRC Press an imprint of Taylor & Francis Group, an Informa business

No claim to original U.S. Government works Version Date: 20140826

International Standard Book Number-13: 978-1-4822-3160-1 (eBook - PDF)

This book contains information obtained from authentic and highly regarded sources. Reasonable efforts have been made to publish reliable data and information, but the author and publisher cannot assume responsibility for the validity of all materials or the consequences of their use. The authors and publishers have attempted to trace the copyright holders of all material reproduced in this publication and apologize to copyright holders if permission to publish in this form has not been obtained. If any copyright material has not been acknowledged please write and let us know so we may rectify in any future reprint.

Except as permitted under U.S. Copyright Law, no part of this book may be reprinted, reproduced, transmitted, or utilized in any form by any electronic, mechanical, or other means, now known or hereafter invented, including photocopying, microfilming, and recording, or in any information storage or retrieval system, without written permission from the publishers.

For permission to photocopy or use material electronically from this work, please access www. copyright.com (http://www.copyright.com/) or contact the Copyright Clearance Center, Inc. (CCC), 222 Rosewood Drive, Danvers, MA 01923, 978-750-8400. CCC is a not-for-profit organization that provides licenses and registration for a variety of users. For organizations that have been granted a photocopy license by the CCC, a separate system of payment has been arranged.

Trademark Notice: Product or corporate names may be trademarks or registered trademarks, and are used only for identification and explanation without intent to infringe.

Visit the Taylor & Francis Web site at http://www.taylorandfrancis.com

and the CRC Press Web site at http://www.crcpress.com

For information about Apple Academic Press product http://www.appleacademicpress.com

ABOUT THE EDITOR



Mihai V. Putz, PhD

Mihai V. Putz is a laureate in physics (1997), with an MS degree in spectroscopy (1999), and PhD degree in chemistry (2002), with many post doctorate stages: in chemistry (2002-2003) and in physics (2004, 2010, 2011) at the University of Calabria, Italy, and the Free University of Berlin, Germany, respectively. He is currently Associate Professor of theoretical and computational physical chemistry at West University of Timisoara, Romania.

He has made valuable contributions in computational, quantum, and physical chemistry through seminal works that appeared in many international journals. He has actively promoted new method of defining electronegativity, DFE (density functional electronegativity) among new enzyme kinetics (logistic enzyme kinetics), a new formalization of the structure-activity relationship (SPECTRAL-SAR) model and recently the bondonic quasi-particle theory of the chemical bonding first application on nanosystems as graphene, all seeking for a unitary quantum approach of the chemical structure and reactivity targeting the bio-, pharmaco- and ecological analytical description.

He is Editor-in-Chief of the *International Journal of Chemical Modeling* and the *International Journal of Environmental Sciences*. He is member of many professional societies and has received several national and international awards from the Romanian National Authority of Scientific Research (2008), the German Academic Exchange Service DAAD (2000, 2004, 2011), and the Center of International Cooperation of, Free University Berlin (2010). He is the leader of the Laboratory of Computational and Structural Physical Chemistry for Nanosciences and QSAR at the Biology-Chemistry Department of West University of Timisoara, Romania, where he conducts research in the fundamental and applicative fields of quantum physical-chemistry and QSAR. In 2010 Mihai V. Putz was declared through a national competition the Best Researcher of Romania; in 2013 he was recognized among the first Dr. Habil in Chemistry in Romania, and from 2014 he became full member of International Academy of Mathematical Chemistry (IAMC).

This page intentionally left blank

CONTENTS

	List of Contributorsix
	List of Abbreviationsxi
	List of Symbolsxiii
	Preface
	Forewordxxi
1.	Nanouniverse Expanding Macrouniverse: From Elementary Particles to Dark Matter and Energy1
	Mihai V. Putz
2.	Inerton Field Effects in Nanosystems
	Volodymyr Krasnoholovets
3.	Non-Classical Properties of Classical Nanostructures
	Jan C. A. Boeyens
4.	Exotic Multi-Shell Nanostructures
	Mircea V. Diudea
5.	The Self-Assembly of Porphyrin Derivatives into 2D and 3D
	Architectures
	Mihaela Birdeanu and Eugenia Fagadar-Cosma
6.	Recent Trends in Nano-Optomechanical Systems 207
	Aranya B. Bhattacherjee, Neha Aggarwal, and Sonam Mahajan
7.	Magnetic Anisotropy in Case Studies
	Marilena Ferbinteanu and Fanica Cimpoesu
8.	Functional Supramolecular Systems Controlled by Light
	Tommaso Avellini Massimo Baroncini Enrico Marchi Monica Semeraro, and Margherita Venturi
9.	Novel Parallel Stacking Interactions of Aromatic Molecules
	Dušan P. Malenov and Snežana D. Zarić
10.	Nanochips for Mass Spectrometry and Applications in Biomedical Research
	Alina D. Zamfir

11.	The "How-To" Guide to Computational Crystallography 4	
	Emre S. Tasci, Alessandro Stroppa, Domenico Di Sante, Gianluca Giovannetti, Silvia Picozzi, and J. Manuel Perez-Mato	
	Index	

LIST OF CONTRIBUTORS

Neha Aggarwal

Department of Physics and Astrophysics, University of Delhi, Delhi - 110007, India

Tommaso Avellini

Dipartimento di Chimica "Giacomo Ciamician", Università degli Studi di Bologna, Via Selmi, 2 - 40126, Bologna

Massimo Baroncini

Dipartimento di Chimica "Giacomo Ciamician", Università degli Studi di Bologna, Via Selmi, 2 - 40126, Bologna

Aranya B. Bhattacherjee

Department of Physics, ARSD College, University of Delhi (South Campus), New Delhi-110021, India

Mihaela Birdeanu

National Institute for Research and Development in Electrochemistry and Condensed Matter, 1 Plautius Andronescu Street, 300224 Timisoara, Romania

Jan C. A. Boeyens

Unit for Advanced Scholarship, University of Pretoria South Africa

Fanica Cimpoesu

Institute for Physical Chemistry, Splaiul Independentei 202, Bucharest 060021, Romania

Eugenia Fagadar-Cosma

Institute of Chemistry Timisoara of Romanian Academy, 24 M Viteazu Ave., 300223-Timisoara, Romania

Mircea V. Diudea

Department of Chemistry, Babes-Bolyai University, Arany Janos 11, 400028, Cluj, Romania

Marilena Ferbinteanu

University of Bucharest, Faculty of Chemistry, Inorganic Chemistry Department, Dumbrava Rosie 23, Bucharest 020462, Romania

Gianluca Giovannetti

CNR-IOM-Democritos National Simulation Centre and International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136, Trieste, Italy

Volodymyr Krasnoholovets

Indra Scientific, Square du Solbosch 26, B-1050 Brussels, Belgium

Sonam Mahajan

Department of Physics and Astrophysics, University of Delhi, Delhi - 110007, India

Dušan P. Malenov

Department of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, Serbia

Enrico Marchi

Dipartimento di Chimica "Giacomo Ciamician", Università degli Studi di Bologna, Via Selmi, 2 - 40126 Bologna

J. Manuel Perez-Mato

Dept. Fisica de la MateriaCondensada, Fac.Ciencia y Tecnologia, Universidad del Pais Vasco, UPV/ EHU 48080 Bilbao, Spain

Silvia Picozzi

CNR-SPIN, L'Aquila, Italy

Mihai V. Putz

Laboratory of Computational and Structural Physical Chemistry for Nanosciences and QSAR, Biology-Chemistry Department, Faculty of Chemistry, Biology, Geography, West University of Timişoara, Pestalozzi Street No.16, Timişoara, RO-300115, Romania

Domenico Di Sante

University of L'Aquila, Physics Department, Via Vetoio, L'Aquila, Italy

Monica Semeraro

Dipartimento di Chimica "Giacomo Ciamician", Università degli Studi di Bologna, Via Selmi, 2 - 40126 Bologna

Alessandro Stroppa

CNR-SPIN, L'Aquila, İtaly

Emre S. Tasci

Physics Dept. Middle East Technical University, METU 06800 Ankara, Turkey

Margherita Venturi

Dipartimento di Chimica "Giacomo Ciamician", Università degli Studi di Bologna, Via Selmi, 2 - 40126 Bologna

Alina D. Zamfir

Faculty of Physics, West University of Timisoara, Romania, Plautius Andronescu nr. 1, 300224, Timisoara, Romania

Snežana D. Zarić

Department of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, Serbia

LIST OF ABBREVIATIONS

AFM	Atomic Force Microscopy
AU	Astronomic Unit
BEC	Bose Einstein Condensate
CASSCF	Complete Active Space Self Consistent Field
CE	Capillary Electrophoresis
CID	Collision-Induced Dissociation
CNS	Central Nervous System
CRM	Charge Residue Model
CSD	Cambridge Structural Database
DFT	Density Functional Theory
DNP	Dioxynaphthalene
DRIE	Deep Reactive Ion Etching
ECD	Electron Capture Dissociation
EOF	Electroosmotic Flow
ETD	Electron Transfer Dissociation
GS	GroundState
GUT	Grand Unification Theory
НСТ	High Capacity Ion Trap
HG	Hydrodynamic Laws of Gravity
HPLC	High Performance Liquid Chromatography
IR	Infrared
IRMPD	Infrared Laser Multiphoton
LB	Langmuir-Blodgett
LIF	Laser Induced Fluorescence
MCP	Microchannel Plate
MLCT	Metal-to-Ligand (BPY) Charge-Transfer
MRI	Magnetic Resonance Imaging
MS	Mass Spectrometry
NMS	Normal Mode Splitting
OMC	Optomechanical Crystal
PYI	Pyrene Ligand
Q.C.D.	Quantum Chromodynamics
QD	Quantum Dots (Nanocrystals)

SCM	Single Chain Magnets
SEM	Scanning Electron Microscopy
SIM	Single Ion Magnets
SMM	Single Molecule Magnet
SORI	Sustained Off-Resonance Ion
SPM	Scanning Probe Microscopy
STM	Scanning Tunneling Microscopy
TDC	Time to Digital Converter
TGR	Theory of General Relativity
TIC	Total Ion Current
TLC	Thin-Layer Chromatographic
TOE	Theory of Everything
TOF	Time-of-Flight
ТОРО	Trioctyl Phosphine Oxide
TTF	Tetrathiafulvalene
UHV	Ultra-High Vacuum
WMAP	Wilkinson Microwave Anisotropy Probe
XIC	Extracted Ion Chromatogram
ZFS	Zero Field Splitting

LIST OF SYMBOLS

Λ	amplitude of the inerton cloud of the NTH node
δr_{n}	deviation of this node from its equilibrium position
dS	element of space-time
$d\Psi(w)$	extension of 3D
$ u_0$	initial velocity of the particle
g	lattice vector
μ_0	mass of the excited cloud of inertons
m _n	mass of the n-th node
T_{v}	neutrinos temperature
\vec{B}	outer field
$p_0 = m v_0$	particle's initial momentum
т	particle's mass
\overline{T}	period of collision
$\kappa = \Gamma / 2$	phonon damping rate
l p	Planck length
χ	position of the centre mass of the (quantum) cloud
\hat{S}_A	spin operators
\dot{r}_{tan}	tangential velocity of a test mass
$V^{\mathrm{deg.\ cell}}$	typical average volume of a cell
μ_{n}	variations of mass of n-th node
V ^{part}	volume of the kernel cell of the particle
η	viscosity
$m_{_{B}}$	Bohr magneton
ພື	unperturbed cyclotron frequency
μ_{e}	electrophoretic mobility
μ_{eof}	mobility of the electroosmotic flow
\vec{r}, \vec{R}	collection of the electronic and ionic degrees of freedom
$\hat{n}(\vec{r})$	density operator
" "	parallel orientation
···"	denotes hydrogen bonding
1/T	frequency of collisions
A _{in1}	input noise operators for the two optical modes

с	speed of light
D	effective parameters
D ₀₂	initial inner diameter
e	Bouligand exponent
Ε	energy of the moving particle
F _x	x component of atomic spin
Ψ	GS (Ground State) of the system
h	Planck's constant
$J_{_{AB}}$	coupling constants
K	number of repeating units
K _B	Boltzmann constant
M	metal atom
N_a	unpaired electrons
P	pentagon
Q	ionic charge
R	ionic radius
Sz	collective spin operators of the BEC
t^{-}	time
U_{ab}	inter-center Coulomb repulsion term
V _{ee}	electron-electron interaction
X	scaling factor
Y_{lm}	Spherical Harmonics
Ζ	combination of spherical harmonics
Γ	force constant
$\Delta E_{HOH/HOH}$	energy of interaction between water molecules
Ξ	noise operator arising as the mechanical mode
γ	atomic damping rates
γ_1	angles
$\Omega_{\rm r}$	mechanical frequency of the cantilever mode

PREFACE

With the dawn of the 21st century, the need for new sources of energy and the increased demand for economical and multifunctional materials in the fields of mechanics, electronics, medicine, and ecology becomes more and more acute as natural, physical, and chemical resources (natural energy and fuels) reveal their limits, their difficulties, and their increased costs in storage, transport, and conversion. Therefore, knowledge of the universe and its materials (along with their self-assembly, self-regeneration, storage, and directional properties) are on the forefront of fundamental and technical research worldwide, in both academia and industry. In response to these challenges, the scientific community has developed the required synergy among involved fields, and the nanosciences emerged, aiming to combine and transfer knowledge (models, tools, practical support) from physics to chemistry to biology and related fields, producing a unitary view of how nano-phenomena trigger micro and macro cosmos, observable or hidden, and designed actions and materials to be implemented toward optimizing everyday life and secure its future.

As a consequence, new phenomena and exotic materials and properties are being explored in current research horizons. These include the quantum universe from the nano- to large-scale understanding in general, with applied subdomains at molecular levels, such as, for example:

- · topological effects in nanosystems
- · nanostructured solar cells
- · noncovalent interactions in organometallic chemistry
- spin crossover compounds
- hysteresis in molecular magnets
- · structure anistropy and related properties
- · organic ferroelectrics
- · coordinative chemistry of actinide ions
- modeling of bioinorganic materials
- nanoscience of carbon's allotropes (fullerenes and nanotori, self-assembly structures, new diamonds, and spongy-carbon; new theorems, tessellation, and aromaticity modeling, chemical reactivity of fullerenes)

These new research horizons also include chemistry and nanoscience and chemical nanostructures from structure to properties such as, among many others:

- · oxa- and oxaaza-coronands
- · nano-electronics and nano-devices
- nanobiomaterials for dentistry (such as new highly fluorescent materials, chemical captors, chemosensors)
- · nanoscience of textiles, food, and ecotoxicology
- · optical properties control and design of multifunctional nanomaterials

These topics viewed together assure a consistent picture of matter from quantum particles to atoms and molecules and to solid state, bonded at nanoscale, while manifesting meso to macro effects.

This book aims to collect and order the physical and chemical perspectives on nanosystems triggering macrosystems from a wide perspective of cosmic phenomenas to special nano-devices and phenomena in a succession of chapters narrating "the story of observable and induced cosmos through the eyes of nano-particles and devices."

Chapter 1 presents the so-called Fermi calculations (smart calculations), the fundamental relations of environmental large-scale physics by considering the space-time-energy properties of light and of its quantum photon; from the black-body radiation and light pressure, one may make predictions associated with the quantification of dark mass and energy in the universe, balancing between Jeans' contraction of galaxies and Hubble's expansion.

Chapter 2 describes the universe of particles and their motion as based on a mathematical space constructed as a tessellation lattice of primary balls, while the motion of a particle generates a cloud of excitations around the particle, which were named *inertons*, with remarkable consequences in treating the quantum ψ -function as a mapping of the real system "particle + its cloud of inertons." The basic feature of inertons, that is, is both the particles' inert and gravitational properties, which assures their observability in diluted cold gases and clusters of electrons, or by the Casimir effect; whereas through the associated electromagnetic field, it is able to give a deeper insight into the fundamental nature of things, playing an important role in quantum physics, chemical physics, biochemistry, biophysics, and condensed matter.

Chapter 3 surveys the limits of classical quantum mechanics because the inherent embedded linearity in the basic theory; in addition it is argued that nonlinearity plays a major role in the universe in general and in the nano-materials and scales in particular, such as, for example, the major types of

nanoparticles, including nanogold, graphene, fullerene, boron nitride, semiconductors, and their derivatives. This observation, along with the need for a description of a 4D universe, which implies descriptive geometry alike, proposes a critical understanding and modeling of the nonclassical properties of nanomaterials through number theory and universal self-similarity.

Chapter 4, instead, takes the topological route to describe the nanoworld structures: as constructive units, small cages are used to design complex structures of rotational or translational symmetry, whereas the design of multishell cages recalls the Platonic solids and their transforms, obtained by using simple map operations. The celebrated quasicrystals structures are in this way recovered by self-arrangements and multishell combinations, whereas genus and Omega polynomial calculations enrich the structure characterization of these exotic structures under the spongy manifestation.

Chapter 5 continues the observations of the previous chapter in the selfarranging feature of nanostructures by describing through atomic force microscopy (AFM) of the self-assembling porphyrins by weak Van der Waals forces or hydrophobic effects, hydrogen bond and π - π stacking interactions that finally generates a large variety of their geometries. In this way AFM evidences how the J-aggregates (edge-to-edge stacked) and H-bonding interactions are both responsible for generating different architectures, which sometimes coexist together, such as triangle type sheets, concave-convex surfaces, columns, pyramids, roofs, and even rings.

Chapter 6 takes further the use of nanosystems into optomechanical effects: apart from discussing interesting quantum phase transition in a hybrid optomechanical as a selective tool for transfer energy between a single mechanical mode and two optical modes, an advanced idea of producing laser modes of phonons by the aid of Bose-Einstein condensates is presented and documented, with switching channels controlled by adding atoms into condensate, by magnetically coupling between mechanical oscillations of a nanoscale magnetic cantilever to an ultra-cold atomic cloud in close analogy to a two-level optical laser system.

Chapter 7 presents a survey on today's hot topic of molecular magnetism related with magnetic anisotropy—a phenomena appearing by the interplay of spin and orbital magnetic moments so that obtaining systems behave as magnets at molecular and nano-scale systems. In this framework it presents the pioneering tool for revealing the poles of molecular magnets known as state-specific magnetization surfaces, with specific applications on the f-transition metal ions and d-f complexes, since revealing non-*aufbau* configuration and weak interaction with ligands and neighbor magnetic sites.

Chapter 8 is dedicated to supramolecular photochemistry or more specifically to the design and construction of nanoscale devices and machines capable of performing useful light-induced functions aiming for, in the short run, the transportation of nanoobjects, mechanical gating of molecular-level channels, and nanorobotics, while targeting the construction of chemical computers nano-scale research in the long run. From energy (solar) conversion to sensoring and catalysis, other viable supramolecular photochemistry possibilities include deposition on surfaces, incorporation into polymers, organization at interfaces, or immobilization into membranes or porous materials, providing an open field for still unpredictable challenging nano-functionalizations of materials in interaction with light.

Chapter 9 addresses new systematic insight on aromatic rings interacting with substantial energy at a very large parallel displacement (offsets), out of the ring, even beyond the C-H bond region, and also when the two rings are almost non-overlapping. Accordingly, the noncovalent interactions were explored and their consequences on the nanosystems, aromatic here, are exposed.

Chapter 10 reveals the many facets of chip systems not only in the life sciences but especially on biomedical research. Great relevance is attributed to the research on several micro- and nanofluidics analyzed by using electrospray ionization mass spectrometry (MS). In this regard the mass spectrometry technique and the allied methods (e.g., quadruple time-of-flight (QTOF), Fourier transform ion cyclotron resonance (FTICR), and high capacity ion trap (HCT) are introduced in glycomics for biomedical and clinical frontier applications, such as from screening, sequencing, and the structural analysis of *O*-glycopeptides expressed in the urine of patients suffering from Schindler's disease versus age-matched healthy controls leading to de novo design and validation of useful biomarkers.

Chapter 11 completes the book with a didactic-research exposé on how computational crystallography may use the celebrated density functional theory in studying the ferroelectric properties of materials.

As such, this book is both multidisciplinary and transdisciplinary: it combines methods from various physicochemical fields and presents novel paradigms from one discipline to be applied or transferred to other disciplines, thus offering new insights that apply to various physicochemical, biophysical, biochemical, etc., fields at nano- and mesoscales.

With chapters written by leading international scientists, the book balances both experimental results and theoretical modeling, and the new cutting research trends discussed will be equally valuable to both academia and industry.

Altogether, *Quantum Nanosystems: Structure, Properties, and Interactions* benefits from 21st-century knowledge in the nanosciences, making it pivotal in helping to open new frontiers and research horizons for understanding, synthesizing, and using matter at nanoscale (atoms and molecules) to advance the self-adapted multifunctional use and know-how of nanosystems for new energy, new materials, new technology, and new ecology.

Written by leading and open-minded scientists with international reputations, the book should be in every library of nanoscience literature. This book is enriched by the contributions from leaders from various fields, ages, and countries, all with international research experience and highly rated publications to their credit. It covers a wide and advanced variety of issues and open-issues in nanosciences. The Editor, knowing personally almost all of the contributors, has a vivid interest in connecting their fields of discipline. True thanks are offered to all the contributing authors for their dedication and high-level expertise and for helping to advance 21st-century science beyond the customary frontiers of physics, chemistry, and engineering. Equally, the Editor gratefully acknowledges the research and editing facilities provided by the Romanian Education and Research Ministry within the project CNCS-UEFISCDI-TE-16/2010-2013. Last but not least, the Editor, also on behalf of the book's contributors, thanks the Apple Academic Press team and, in particular, Ashish Kumar, president and publisher, for professionally supervising the production of the multidisciplinary scientific series in general and of this volume in particular.

— Mihai V. Putz, PhD

(Assoc. Prof. Dr. Habil) West University of Timişoara, Romania April 2014 This page intentionally left blank

FOREWORD

The latest generation of optomechanical quantum systems based on Bose Einstein condensates properties, phonon lasers, light-controlled molecular machines—the building blocks for the next-decade supramolecular photochemistry, and the most recent developments of ab-initio computational crystallography are reported here in association with more "imaginative" chapters as well, devoted to Coxeter-like atlas of novel hyperstructures or to the intriguing description of *inerton field* and the way it influences the basic properties of the matter. Outcomes of several important research studies are presented in these well-written chapters. Detailed descriptions of magnetic anisotropy phenomena and porphyrin derivatives characterized by atomic force microscopy imaging are enriched by deep insights on the emerging role of non-covalent interactions in determining the nanostructure of aromatic rings stacking.

Prof. Putz keeps a balanced eye on nanoscale on applicative and fundamental subjects, prompting graduates students and professional researchers on the latest theoretical results. Fibonacci decorations on the surface of Ag/ silica particles disclose a profound theoretical re-examination of the growing mechanisms of "nanoparticles," from nanogold to semiconductors, evidencing how much quantum systems are conditioned by their inherent *fourdimensional nature*. The instrumental service of quantum theories in shaping micro- and macro- cosmos is testified the editor's original investigation on the spatial-temporal evolution of the universe resulting in an appropriate estimate of the dark matter vs. dark energy observed distribution, which captures the reader's attention on the inextricable, scale-invariant efficiency of the physical laws in describing the world.

The outstanding scientific level of the authors contributing to this book simply makes these "horizons" a must-read book on nanomaterials.

This volume constitutes an authoritative guide to nanoworld and will surely support frontier research in chemical physics, biochemistry, biophysics, condensed matter, and modern quantum theory as well.

> Ottorino Ori Actinium Chemical Research Rome, September 9, 2013

This page intentionally left blank

NANOUNIVERSE EXPANDING MACROUNIVERSE: FROM ELEMENTARY PARTICLES TO DARK MATTER AND ENERGY

MIHAI V. PUTZ

CONTENTS

Abs	tract	2
1.1	Introduction	2
1.2	Background Theories of Universe	3
1.3	Fermi-Weinberg Type Estimations of Universe Dark Matter	
	and Energy	
1.4	Conclusion	49
Ack	nowledgments	49
Key	words	50
Refe	rences	50

ABSTRACT

"Fermi calculations" (smart calculations) for the combination of the fundamental relations of the environmental physics at large scale are considered in determining of the space-time-energy quantities of practical interest broadening the general knowledge of macro-cosmos based on the micro/nano matterproperties; to this aim, the existence of the photon and the associated (black body) radiation is explicitly or implicitly involved, according to the occurrence of the measures directly observed or through the estimated effect produced by Universe after the first milliseconds (in the era of nucleo-synthesis, nuclei, atoms and galaxies). This way, the predictions associated to the quantification of dark mass and energy are made for a Universe associated to the Jeans contraction of galaxies and to the Hubble expansion, respectively.

1.1 INTRODUCTION

In order to offer classical-quantum unitary view of the phenomena of macromicro-cosmos, this chapter combines three fundamental themes of Physics, such as, Classical Mechanics with applications to the gravitational Newtonian mechanics; Relativistic Mechanics with the Einstein kinematic forms and consequences, with application in description of the Universe in expansion through Hubble's law, the argument for the Big-Bang Theory; statistical Physics with Bose-Einstein distribution, with applications and consequences of the radiation of black body at the level of the Universe and the elementary particles.

These themes and the related applications have been selected (from the author's experience by teaching topics of Environmental Physics) as being the most accessible and useful to the students who are in direct contact with the Modern Physics, with applications and universal models, related to the forces and fundamental particles, stars and planets, nuclear reactions and radioactive decay, while accumulating imperative notions to future approaches of modeling the Structure of the Atoms and Molecules, Structural Physical-Chemistry, Quantum Chemistry and Environmental Chemistry of course.

It was purposely omitted the presentation of other universally theory which naturally arising from the presented arguments—*The General Theory of Relativity*—which, although very important for a complete description of Cosmology (at least in terms of gravity, or precisely in terms of the principle of equivalence inertial mass-gravitational mass, sustained by the expansion of physical laws beyond the inertial systems to the accelerated systems) it would enlarge to much of this chapter, which only contains the essential cosmological ideas and determinations: Bing Bang modeling through the straight after zeroth moment—Planck Universe, Expansion of Universe, calculations of Expansion time while the Universe become cold, Radiation of Cosmic Background simulation, the quantum-gravity equivalence of photon, etc. As for the General Relativity themes, it was decided to approach it with further occasion, designed precisely for Advanced Environmental Physics.

Therefore, this chapter is made to be a basic, orientate application of the essential principles from Mechanical Physics (classical and quantum), Nuclear and Statistical (classical and quantum), for a better understanding of Universe. Actually, the Environmental Physics can be considered as being not a specific field of Physics, but the fundamental synthesis of all of the Physics chapters, having as a starting point the combination of micro- and macro-phenomena in characterization of global and local observed effects. This "art" to combine micro- and macro-cosmos is actually one of the conceptual, didactic and scientific challenge (attribution) of Environmental Physics at a classical-quantum-relativistic combined level.

The fascination and sometimes the difficulty of this subject appear when the quantities of the micro universal constants (light speed in vacuum and Planck constant) are combined with the macro ones (as the universal gravitational constant or Boltzmann constant for a statistical ensemble to the macroscopic balance type) in order to generate physical sizes (length, time, temperature, etc.) with universal value; but definitely they give the unifying key in the right knowledge, prediction and even the control of the evolution and interactions of Nature's objects.

Thus, this chapter is dedicated especially to those from Physics related specializations and interdisciplinary applications in environmental problems; yet, this chapter can be also read and used as a model-guide in combining the fundamental notions of Physics by the graduate students. Furthermore, it can be used in the Scientific Cycles and the extracurricular activities of preacademic intermediate, but also as a starting point in writing a graduation paper, in Physics and Chemistry, regarding the Cosmology and considering the Universe as an open physical system.

1.2 BACKGROUND THEORIES OF UNIVERSE

1.2.1 ON GRAVITATION AND GALACTIC CONDENSATION

One starts by observing the gravitational attraction law can be written under gradient formulation

$$\dot{F} = m \cdot \vec{g} = -m \cdot gradU \tag{1}$$

with gravitational potential given by the simple expression

$$U = -G\frac{M}{r} \tag{2}$$

Worth noting that the Eq. (2), through which the dynamic (inertial) form is equalized with the gravitational form of Newton's law, represents the premise of the so-called principle of equivalence (between the inertial mass and the gravitational mass), fundamental for the general relativity theory of Einstein! In these conditions, one can apply the Gauss's law/theory which connects the flow of a vector \vec{g} , through a closed surface Σ , to the divergence integral.

$$\oint_{\Sigma} \vec{g} d\vec{S} = \int_{V} div \vec{g} dV$$
(3)

If we consider the vector in question as being bound to the gravitational source of Newton's attractive force,

$$\left|\vec{g}\right| = \left|grad_{r}U\right| = \left|\nabla_{r}\left(G\frac{M}{r}\right)\right| = G\frac{M}{r^{2}}$$
(4)

then, the left side of Gauss's law term in Eq. (3) is consecutively written

$$\oint_{\Sigma} \vec{g} d\vec{S} = \oint_{\Sigma} |\vec{g}| \cos(\vec{g}, \vec{u}_n) dS = -\oint_{\Sigma} |\vec{g}| dS_n = -\int_{\Sigma} |\vec{g}| r^2 d\Omega$$
$$= -GM \int_{\Sigma} d\Omega = -4\pi GM = -4\pi G \int_{V} \rho dV$$
(5)

where the natural geometry from Fig. 1.1 have been considered for the scalar product of gravitational acceleration with the unit vector (normal at the integration surface).



FIGURE 1.1 Geometry of gravitational action for Gauss's law application for gravitational acceleration; credit: Putz, M.V. Environmental Physics and Universe (in Romanian as "Fizica Mediului și Universul") West University of Timișoara Press: Timișoara, 2010 (adapted after HyperPhysics 2010; http://hyperphysics.phy-astr.gsu.edu/hbase/hph.html).

By equalizing the last result with the right side of Gauss's law (3) the relation of gravitational acceleration divergence results

$$div\bar{g} = -4\pi G\rho \tag{6}$$

In terms of gravitational potential gradient, the last relation is written first by a direct replacement

$$div(-gradU) = -4\pi G\rho \tag{7}$$

which is immediately generated by recognizing the differential identity involving the Laplacin of the gravitational potential

$$div(gradU) = \vec{\nabla} (\vec{\nabla} U) = \nabla^2 U = \Delta U , \qquad (8)$$

and the Poisson's theorem for propagation of gravitational potential based on the gravitational source represented by the mass density ρ

$$\Delta U = 4\pi G\rho \tag{9}$$

equivalent with the Newton's law of gravitational action at a distance! Moreover Poisson's gravity equation usually represents the benchmark and the classical nonrelativistic specialization of Einstein's equations of Theory of General Relativity (TGR).

Notice that, because the gravitational field is not a closed field inside the producing source volume, the gravitational acceleration corresponds to a non-rotational field, which, in terms of field equation is rewritten by canceling the associated rotor

$$rot\vec{g} = \nabla \times \vec{g} = 0 \tag{10}$$

As an application to the Universe structure, the law of gravitational acceleration divergence will be further used, in order to elaborate the classical model (nonrelativistic and nonquantum) of the cosmic systems, galaxies, stars and planets formation.

We consider the gravitational field as a fluid, which follows the hydrodynamic laws. Considering the gravitational source as being represented by the mass density ρ , the gravitational field is moving with a velocity \vec{v} , with the gravitational acceleration \vec{g} oriented to the center of the mass source and developing a pressure \vec{P} reactive to the gravitational effect (i.e., contrary to this); it satisfy three forms of hydrodynamic laws of gravity (HG):

The continuity of gravitational charge equation, which varies in space and time in a given region

HG1:
$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \underbrace{(\rho \vec{v})}_{\substack{GRAVIFIC\\CHARGE\\CURRENT}} = 0$$
 (11)

The convective hydrodynamic equation HG2 of total gravitational acceleration equation written as the (absolute) convective derivative

$$\frac{D\vec{v}}{Dt} = \frac{d}{dt}\vec{v}\left(t,\vec{x}(t)\right) = \frac{d\vec{v}}{dt} + \frac{d\vec{v}}{dx}\frac{d\vec{x}}{dt} = \frac{d\vec{v}}{dt} + \left(\vec{v}\cdot\vec{\nabla}\right)\vec{v}$$
(12)

resulted from the competition between the gravitational acceleration of the source and the one generated from the reactive pressure of the gravitational field (which can be of quantum nature if it's referring to the photons pressure radiated by a star, or purely of kinetic nature if it's referring to galactic or cosmic gas dust which condenses)

HG2:
$$\frac{d\vec{v}}{dt} + (\vec{v} \cdot \vec{\nabla})\vec{v} = -\frac{\vec{\nabla}P}{\rho} + \vec{g}$$
 (13)

The equation of gravitational flux, connected to the gravitational acceleration divergence (and by default to the Poisson form of Newton gravitational law):

HG3:
$$\nabla \cdot \vec{g} = -4\pi G \rho$$
 (14)

Then, one considers as an initial state (unperturbed) of the galactic/stellar/ planetary structure the intergalactic space (-stellar or -planetary), where the gravity forces and masses are absent, i.e. the mass density and pressure being constant quantities Nanouniverse Expanding Macrouniverse

$$\begin{array}{l}
\text{INITIAL} \\
\text{GALACTIC} \\
\text{STATE} \\
\end{array} \begin{cases}
\vec{g} = \vec{g}_0 = 0 \\
\vec{v} = \vec{v}_0 = 0 \\
\rho = \rho_0 = ct. \\
P = P_0 = ct.
\end{array}$$
(15)

The formation of galactic nebulae, stellar or planetary, is thus considered to be associated with the bringing of gravitational forces in a perturbative way, where the previous conditions become

$$\begin{array}{l}
\left| \vec{g} = \vec{g}_{1} \\
\vec{v} = \vec{v}_{1} \\
\left| \vec{v} = \rho_{0} + \rho_{1} \dots \rho_{1} / \rho_{0} \in [-1, +1] \\
P = P_{0} + P_{1} \dots P_{1} / P_{0} \in [-1, +1] \\
\end{array} \right| \tag{16}$$

which lead to the specialization of the hydrodynamic equations of gravity. Thus, HG1 becomes *galactic*-HG1 (GHG1) equation

$$\frac{\partial \rho_0}{\partial t} + \frac{\partial \rho_1}{\partial t} + \vec{\nabla} \cdot \left[\left(\rho_0 + \rho_1 \right) \cdot \vec{v}_1 \right] = 0$$

$$\Leftrightarrow \frac{\partial \rho_1}{\partial t} + \rho_0 \vec{\nabla} \cdot \vec{v}_1 + \frac{\rho_1}{\Xi 0} \vec{\nabla} \cdot \vec{v}_1 + \vec{v}_1 \vec{\nabla} \cdot \frac{\rho_1}{\Xi 0} = 0$$

$$\Longrightarrow \text{GHG1:} \quad \frac{\partial \rho_1}{\partial t} + \rho_0 \vec{\nabla} \cdot \vec{v}_1 = 0 \quad (17)$$

In same manner, HG2 becomes GHG2:

2

~

$$\frac{d\vec{v}_1}{dt} + \left(\vec{v}_1 \cdot \vec{\nabla}\right) \underbrace{\vec{v}_1}_{\equiv \vec{0}} = -\frac{\vec{\nabla} \cdot \left(P_0 + P_1\right)}{\rho_0 + \rho_1} + \vec{g}_1$$
$$\Leftrightarrow \frac{d\vec{v}_1}{dt} \cong -\frac{\vec{\nabla} P_1}{\rho_0} + \vec{g}_1 \tag{18}$$

If the size is introduced by taking the pressure divergence,

$$\vec{\nabla}P_1 = \frac{\partial P_1}{\partial \rho_1} \frac{\partial \rho_1}{\partial x} = v_S^2 \vec{\nabla} \rho_1 \tag{19}$$

connected with the sound speed in gravitational matter

$$v_S = \sqrt{\frac{\partial P_1}{\partial \rho_1}} \tag{20}$$

we obtain the following expression for the GHG2 law

$$\frac{d\vec{v}_1}{dt} \approx -\frac{v_S^2}{\rho_0} \vec{\nabla} \rho_1 + \vec{g}_1 \tag{21}$$

Next, by calculating the derivative of equation GHG1 in relation with the time and then using the expression GHG2 followed by the integration of equation HG3 one successively obtains

$$0 = \frac{\partial}{\partial t} \left(\frac{\partial \rho_{1}}{\partial t} + \rho_{0} \vec{\nabla} \cdot \vec{v}_{1} \right)$$
$$= \frac{\partial^{2} \rho_{1}}{\partial t^{2}} + \rho_{0} \vec{\nabla} \cdot \frac{\partial \vec{v}_{1}}{\partial t}$$
$$= \frac{\partial^{2} \rho_{1}}{\partial t^{2}} + \rho_{0} \vec{\nabla} \cdot \left[-\frac{v_{S}^{2}}{\rho_{0}} \vec{\nabla} \rho_{1} + \vec{g}_{1} \right]$$
$$= \frac{\partial^{2} \rho_{1}}{\partial t^{2}} - v_{S}^{2} \nabla^{2} \rho_{1} + \rho_{0} \underbrace{\vec{\nabla} \cdot \vec{g}_{1}}_{HG3}$$
$$= \frac{\partial^{2} \rho_{1}}{\partial t^{2}} - v_{S}^{2} \nabla^{2} \rho_{1} - 4\pi G \rho_{0} \rho_{1}$$

generating a single hydrodynamic gravific condensation (HGC) equation

HGC:
$$\frac{\partial^2 \rho_1}{\partial t^2} = v_s^2 \nabla^2 \rho_1 + 4\pi G \rho_0 \rho_1$$
 (23)

(22)

which emphasizes the time variation relating the space modification for the galactic gravitational condensation through mass density of initial galactic state, together with the sound speed in the gravitational mass involved in condensation and with the contribution of universal gravitational constant G.

Nanouniverse Expanding Macrouniverse

Finding a "monochromatic" solution of condensation gravitational density, such as, solves the equation,

$$\rho_1 \propto \exp\left[i(kx - \omega t)\right] \tag{24}$$

By formation of the directly relations

$$\begin{cases} \frac{\partial^2 \rho_1}{\partial t^2} = -\omega^2 \rho_1 \\ \nabla^2 \rho_1 = \frac{\partial^2 \rho_1}{\partial x^2} = -k^2 \rho_1 \end{cases}$$
(25)

the HGC equation (23) is reduced to the relationship of gravitational dispersion of condensation

$$\omega^{2} = v_{S}^{2}k^{2} - 4\pi G\rho_{0}$$

= $v_{S}^{2}\left(k^{2} - \frac{4\pi G\rho_{0}}{v_{S}^{2}}\right)$
= $v_{S}^{2}\left(k^{2} - k_{J}^{2}\right)$ (26)

where the Jeans' wave vector has been introduced

$$k_J = \sqrt{\frac{4\pi G\rho_0}{v_S^2}} \tag{27}$$

This way, we reached the classical interpretation of the galactic condensation phenomena under the action of gravitational force: when the body mass exceeds the mass contained in Jeans' sphere, of radius

$$R_J = \frac{2\pi}{k_J} = \sqrt{\frac{\pi v_S^2}{G\rho_0}}$$
(28)

2/2

beyond the critical Jeans' mass

$$M > M_J = \left(\frac{4}{3}\pi R_J^3\right)\rho_0 = \frac{4}{3}\pi\rho_0 \left(\frac{\pi v_S^2}{G\rho_0}\right)^{3/2}$$
(29)

it leaves with the condition

$$k < k_J \tag{30}$$

with the appearance of imaginary frequencies as the direct consequence

$$\omega_J = \pm i v_S \sqrt{k^2 - k_J^2} = \pm i \operatorname{Im} \omega \tag{31}$$

and respectively with the instability in the solution of mass density

$$\rho_{1} \propto \exp\left[-i\omega_{J}t\right] = \exp\left[\pm|\mathrm{Im}\,\omega|t\right]$$
$$= \begin{cases} \exp\left[+|\mathrm{Im}\,\omega|t\right] \dots \text{ contraction} \\ \exp\left[-|\mathrm{Im}\,\omega|t\right] \dots \text{ aeration} \end{cases}$$
(32)

However, the present theory gives interesting information: the universal gravitational constant G might be seen, by eliminating the mass density in the initial galactic state between the mass and the Jeans' radius, such as

$$G = \frac{4\pi^2}{3} v_S^2 \frac{R_J}{M_J}.$$
 (33)

This form has in "its structure" the critical sizes of condensation and the contribution of speed sound by the condensed substance!

The values of this approach can be proved by applying the expression associated to sound speed (obtained in this case by eliminating the Jeans' mass from the last relation with the Jeans' radius and the initial density of condensation)

$$v_S = R_J \sqrt{\frac{G\rho_0}{\pi}} \tag{34}$$

to the Earth data (referred to the Jeans-critical-stable condition) with radius R = 6378 (km) and mass $M = 5.975 \times 10^{24}$ (kg) we have $\rho_0 = 3M / (4\pi R^2) = 5.5$ g/cm³ for which the reasonable value is obtained

$$v_s \cong 2.17 \,\mathrm{km/s} \tag{35}$$

Nevertheless, the gravitational constant has a decisively contribution to the galaxies, stars and planets formation, and it is essentially for systematically cosmological theory, at any level: classical, relativistic, quantum and combined [1-12].

1.2.2 HUBBLE LAW: EXPANDING OBSERVABLE UNIVERSE

A very important kinematic consequence of the special relativity theory is connected to the temporal Lorentz transformation for the time measured in a system (t'), which uniformly moves with a velocity (v) respecting a system of reference (θx) where the time is measured (t)

$$t' = \frac{t - vx/c^2}{\sqrt{1 - v^2/c^2}}$$
(36)

with *c*-speed of light in vacuum.

Therefore, we can immediately write the chain of equivalent temporal transformations

$$t' = \frac{t - \frac{v}{c^2}x}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{t\left(1 - \frac{v}{c^2}\frac{x}{t}\right)}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{t\left(1 - \frac{v}{c^2}c\right)}{\sqrt{1 - \frac{v^2}{c^2}}} = \frac{t\left(1 - \frac{v}{c}\right)}{\sqrt{1 - \frac{v^2}{c^2}}}$$
(37)

where, in frequencies v = 1/t, reverses as

$$v'_{SOURCE} = v \frac{\sqrt{1 - \frac{v^2}{c^2}}}{\left(1 - \frac{v}{c}\right)} = v_{OBS} \sqrt{\frac{1 + v/c}{1 - v/c}}$$
(38)

This relation is valid also at the wavelengths level $(\lambda = c/v)$ between the source system that emits a radiation (the mobile system) and the observed system which observe it (the stationary system)

$$\lambda_{OBS} = \lambda_{SOURCE} \sqrt{\frac{1 + \nu/c}{1 - \nu/c}} \,. \tag{39}$$

The law allows the calculation of displacing velocities of the massive stars (even of the galaxies) when the displacing in spectrum recorded for the Hydrogen atom, the most abundant element of Universe (99.99%), is known. For example, if the green $(n_1 = 2) - blue (n_2 = 4)$ transition line of Hydrogen is displaced inside the spectrum to the red region at 700 nm when observing a galaxy then we have

$$\lambda_{SOURCE} = \frac{c}{v_{SOURCE}} = \frac{ch}{hv_{SOURCE}} = \frac{ch}{13.6eV(1/2^2 - 1/4^2)} = 486 \,\mathrm{nm}$$
(40)

where the h-Planck's constant have been considered

$$h = 6.626068 \times 10^{-34} \,(\text{m}^2 \,\text{kg/s}) \tag{41}$$

along the Bohr law transition in the spectrum of the Hydrogen atom

$$hv = E_2 - E_1 = R_H \left(\frac{1}{n_1^2} - \frac{1}{n_2^2} \right)$$
(42)

with Rydberg's constant

$$R_H = 13.6eV \tag{43}$$

Turning back, form the relativistic Doppler relation (39) we obtain the equation

$$\left(\frac{\lambda_{OBS}}{\lambda_{SOURCE}}\right)^2 = \left(\frac{700}{486}\right)^2 = 2.075 = \frac{1 + v/c}{1 - v/c}$$
(44)

with the velocity result

$$v = -0.35c$$
 (45)

which indicates the fact that the galaxy is drawing away (the minus sign indicates the back velocity orientation -v) from the observer (whereupon the light signal came with the light speed *c*), which it also justifies the name of recessional velocity. Erwin Hubble, while studying the movement of galaxies, observed that all of them are drawing away from the observer, and among each other, *see* Fig. 1.2.



FIGURE 1.2 Left: interpolation of recessional velocities for Hubble's law determination (according to William C. Keel, The Road to Galaxy Formation, Berlin, Springer, 2007, published in association with Praxis Pub., Chichester, UK. ISBN 3540725342); credit: Wikipedia commons http://en.wikipedia.org/wiki/File:Hubble_constant.JPG continuing the excerpt of the original figure of interpolation of article of Hubble.¹

Those observations caused the advancing of the Universe expansion hypothesis. Considering a cosmic scale factor a(t) which represents the relative expansion of the Universe, sometimes called Robertson-Walker scale factor. With its aid the distance D_t can be connected at the moment *t* after the moment characterized by the distance D_0

$$D_0 = D_t a(t) \tag{46}$$

Worth noting that, because the relation (46) assumes as an effect the space expansion at the dimension D_t towards the earlier one, $D_0 < D_t$, the cosmic factor scale has actually the role of contracting the space-time metric while the expansion, in other words, when applied, it will be considered with minus sign in variation:

$$a(t) \xrightarrow{\partial_t} -\partial_t a(t) \tag{47}$$

Under these circumstances, a galaxy is considered at a certain point at the distance D_t from the observer (found in the present moment), the distance modification in time generates the recessional velocity equation (Hubble's law)

¹Edwin Hubble, A Relation Between Distance and Radial Velocity Among Extra-Galactic Nebulae, *Proceedings of the National Academy of Sciences*, **1929**, vol. 15 no. 3, pp. 168–173.

$$v = \partial_t D_t = \partial_t \left(\frac{D_0}{a(t)}\right) = -D_0 \frac{\left[-\partial_t a(t)\right]}{\left[a(t)\right]^2} = \frac{D_0}{\underbrace{a(t)}_{D_t}} \frac{\partial_t a(t)}{a(t)} = \frac{\partial_t a(t)}{a(t)} D_t = HD_t$$
(48)

where Hubble's parameter has been introduced

$$H(t) = \frac{\partial_t a(t)}{a(t)} \tag{49}$$

it is experimentally estimated as being merely a constant, in fact by the interpolations' slope such as those presented in Fig.1.2 with the values established in Table 1.1.

TABLE 1.1 Values Measured for Hubble's Constant

Year	Value H ₀ (km/s)/Mpc	Observer
2009	74.2±3.6	Hubble Space Telescope
2006	77±11.55	Chandra X-ray Observatory
2001	72±8	Hubble Space Telescope

Considering the astronomic distances in the international units:

- astronomic unit (AU), 1 AU = 149,598,871 km, representing the medium distance between Sun and Earth along a complete Earth orbit;
- one light year—the distance traveled by light (with the light speed) in a year, 1 ly \approx 63,241 AU;
- the parsec—the distance from where an astronomic unit subtends a one arcsecond, 1 pc \approx 206,265 AU.

one may observe that, since the Hubble constant has actually the inverse temporal dimension, by considering its observed average value expressed in sec⁻¹

$$H_0 \sim 2.29 \times 10^{-18} \text{ sec}^{-1}$$
 (50)

it can be concluded that its inverse represents the actual age of the Universe

$$t_{Universe} \cong \frac{1}{H_0} = 4.35 \times 10^{17} \, s = 13.8 [Billion Years]$$
 (51)

Nanouniverse Expanding Macrouniverse

If one considers the Hubble constant as a real constant, the Universe expansion equation will be simply written such as:

$$\frac{dD}{dt} = DH_0 \Longrightarrow D = d_0 \exp(H_0 t)$$
(52)

with d_0 the Universe size at a certain moment. Note that this equation has validity on not so large temporal intervals, when complicated phenomena predicted by the generalized relativity, like dark energy, inflation, etc., do occur. For times relatively closed with the observational one (the current time) can establish, with the aid of Hubble's law, the direct relation between the displacement to the red and the recessional speed.

Therefore, if we reconsider (generalize) the relationship between the distance-observer source and the cosmologic scale factor respective for each state, so having the form

$$\underbrace{D_0 a(t_0)}_{SOURCE} = \underbrace{D_t a(t)}_{OBSERVER}$$
(53)

then, the condition of red-shift can be successively written

$$z = \frac{D_t - D_0}{D_0} = \frac{a(t_0)}{a(t)} - 1 \cong \frac{a(t_0)}{a(t_0) + (t - t_0) \left[-\partial_t a(t) \right]_{t = t_0}} - 1$$
$$= \frac{a(t_0)}{a(t_0) \left\{ 1 - \frac{\left[\partial_t a(t) \right]_{t = t_0}}{a(t_0)} (t - t_0) \right\}} - 1 = \frac{a(t_0)}{a(t_0) \left[1 - (t - t_0) H(t_0) \right]} - 1$$
$$= \frac{1}{1 - (t - t_0) H(t_0)} - 1 = \frac{(t - t_0) H(t_0)}{1 - (t - t_0) H(t_0)} \cong (t - t_0) H(t_0) \cong \frac{D_t}{c} H(t_0)$$
(54)

from where one yields the relationship

$$z \cong \frac{v}{c} \tag{55}$$

once the Hubble's law is applied in the last relation of (54).

Worth to mention the fact that the same dependence between the red-shift and the recessional speed can be also established directly by processing the relativistic Doppler relation

$$z = \frac{\Delta\lambda}{\lambda_{SOURCE}} = \frac{\lambda_{OBS} - \lambda_{SOURCE}}{\lambda_{SOURCE}} = \sqrt{\frac{1 + \nu/c}{1 - \nu/c}} - 1 = \frac{\sqrt{1 + \nu/c} - \sqrt{1 - \nu/c}}{\sqrt{1 - \nu/c}}$$

$$=\frac{2v/c}{\sqrt{1-v/c}\left(\sqrt{1+v/c}+\sqrt{1-v/c}\right)}=\frac{2v/c}{\sqrt{1-v^2/c^2}+1-v/c}\cong\frac{2v/c}{1-\frac{1}{2}\frac{v^2}{c^2}+1-v/c}$$

$$=\frac{v/c}{1-\frac{1}{4}\frac{v^2}{c^2}-\frac{1}{2}\frac{v}{c}} \cong \frac{v}{c} \left(1+\frac{1}{4}\frac{v^2}{c^2}+\frac{1}{2}\frac{v}{c}\right) \cong \frac{v}{c}$$
(56)

where the Taylor development has been considered in the first order

$$(1+x)^a \cong 1+ax \tag{57}$$

while the higher powers of the ratio v/c have been neglected.

Through these two demonstrations (actually equivalent) the intimate connection between the Hubble's law and the Doppler's relativistic effect, as a kinematic consequence of the special relativity theory is confirmed, a fact proved by the experimental observations performed by the light receptions from galaxies and clusters of galaxies, Fig. 1.3. Of great philosophical importance, the red-shift and the Hubble law advance the idea that not even our own galaxy (Milky Way), Fig. 1.4, is not the "Middle of the Universe," but it is situated in an area of the Universe, along with other galaxies and groups of galaxies, forming the so-called Island Universe! This discovery is similar with, or generalizes, the Copernicus' discovery that the Earth is not in the middle of the World, but orbits around the Sun!

Moreover, by corroborating the conclusions related to the Universe expansion, correlated to the red-shift and the age of the Universe as the inverse of Hubble's constant (parameter), Fig. 1.5, one immediately reaches the idea for the existence of a start time moment of the Universe, associated with the Big-Bang state, when all the matter was contracted, wherefrom, due to the universal explosion the Universe is uniformly and isotropically extended (large scale), which is confirmed through the red-shift systematically recorded relatively to all of the astral objects observed [13–30].



FIGURE 1.3 Illustration of red-shift of the farther and farther galactic clusters (the distance is in Mega-"light years," Mly) from the observer (situated on the Earth); credit: http://astronomy.nmsu.edu/astr110/ (July 2013).



FIGURE 1.4 Insular structure of our galaxy, Milky Way; credit: http://www.euhou.net/.



FIGURE 1.5 Homogeneous and isotropic expansion of the Universe predicted from the Big-Bang theory, in agreement with the Hubble's Law of red-shift predicted by the relativistic Doppler effect. The picture of the right-down is taken from the research spatial Wilkinson Microwave Anisotropy Probe (WMAP) and represents the "baby" picture of the Universe at about 3000K of Universe (with warm-red and cold-blue spots); adapted after HyperPhysics 2010 (http://hyperphysics.phy-astr.gsu.edu/hbase/hph.html).

1.2.3 ELEMENTARY PARTICLES AND THE PLANCK UNIVERSE

A subtle level of unification of quantum distribution is referring to: (i) the quality of fermions (semi-integer spin) to characterize the substance aka elementary particles of matter; (ii) bosons (integer spin) are attributed to the particles associated with fundamental fields (implicit to forces) of matter which intercede the interactions between elementary particles. In order to clarify, we further expose the characteristic elementary particles to the fundamental forces of Nature.

1.2.3.1 ELEMENTARY FERMIONS

1.2.3.1.1 SLIGHT FERMIONS: LEPTONS

Three fundamental families/generations of leptons list as:

$$\begin{array}{l}
\mathcal{Q} = -1 \\
\mathcal{Q} = 0
\end{array} \left(\begin{array}{c}
e^{-} \\
\upsilon_{e}
\end{array} \right), \left(\begin{array}{c}
\mu^{-} \\
\upsilon_{\mu}
\end{array} \right), \left(\begin{array}{c}
\tau^{-} \\
\upsilon_{\tau}
\end{array} \right) \tag{58}$$

each generation being a combination of charged lepton connected to the corresponding neutrino lepton (neutral).

 e^- , *the electron*, is the oldest known lepton, discovered by J.J. Thomson in 1897, with *electronic neutrino* v_e anticipated by Ettore Majorana (student of E. Fermi, missing in 1938), theorized by Pauli in 1930 and experimentally discovered in 1956 by Reines and Peierls.

 μ^- , *the muon*, was discovered in 1937 by Anderson (also discoverer of positron) with *muonic neutrino* v_{μ} revealed in 1962.

 τ^- , *triton* (from tritos = the third, in Greek), or *thaon*, is a very high mass lepton (of baryons order- see below) considered a heavy lepton, discovered in 1977 by Peierls with *tritonic* (*thaonic*) *neutrino* experimentally identified in 1990.

1.2.3.1.2 HEAVY FERMIONS: QUARKS

Three fundamental families/generations of quarks list as:

$$Q = +2/3 \\ Q = -1/3 \\ \vdots \\ \begin{pmatrix} u \\ d \\ d \\ wn \end{pmatrix} \begin{pmatrix} c \\ s \\ charm \\ strange \end{pmatrix} \begin{pmatrix} t \\ b \\ top/truth \\ botton/beauty \end{pmatrix}$$
(59)

Quark concept have been introduced by M. Gell-Mann in 1964–65 at CALTECH (although a preprint with similar ideas already existed at CERN from Georg Zweig, who called them as *the asis*), by taking the term from the opera *Finnegans Wake* of James Joyce, quoting: "Three quarks for Muster Mark!".

In 1964 were about 200 particles called elementary, without being systematically explained, until the naive theory (with 3 quarks q=u, d, s) of Gell-Mann; for example, the proton appears as the combination p=3q: *uud*, while the neutron has the structure n=3q=udd.

The strangeness of the name came to emphasize the strangeness of these particles, which have a factionary charge, in fact a subelectronic one!

The combination of *3 quarks qqq* forms the bonded states called baryons (nucleons, hyperons, etc.).

The combination of 2 quarks (one quark and one antiquark) $q\tilde{q}$ generates the bonded states of mesons (for example the mesons π , k, or the *charmonium* particle $J/\psi = c\tilde{c}$).

From leptons and quarks the substance of the matter can be formed, whatever complex it may be.

Nevertheless, recently also appear that the quarks may have, in turn, internal structure!

1.2.3.2 FUNDAMENTAL FORCES

1.2.3.2.1 STRONG INTERACTION

Strong interaction occurs between the baryonic quarks.

It is interceded by the g particle-GLUON (from glue= which bind, in English).

• With s(G)=1 spin.

• With zero rest mass m(G)=0.

The interaction through the gluons is the central subject of quantum chromodynamics (Q.C.D); the *cromo* attribute came from the fact that the gluons are characterized as well by the property called "color," a specific number of quantification: red (r), green (g), blue (b), turquoise (antired \bar{r}), (antigreen \bar{g}), yellow (antiblue \bar{b}), with the associated combinations;

The specific potential is written as

$$V_t = -k_1 \frac{1}{r} + k_2 r = \begin{cases} \infty \dots r \to 0\\ \infty \dots r \to \infty \end{cases}$$
(60)

1.2.3.2.2 ELECTRO-MAGNETIC INTERACTION

It occurs between bodies with electric charge, being intermediated by PHO-TON- γ .

- With $s(\gamma)=1$ spin.
- With zero rest mass $m_0(\gamma)=0$.

It is the subject of quantum electrodynamics (Q.E.D.).

The specific potential is written as

$$V_{EM} = -\frac{1}{4\pi\varepsilon_0} \frac{Q_1 Q_2}{r} \tag{61}$$

1.2.3.2.3 WEAK INTERACTION

It models the transformations between the nucleons, being interceded by WEAKONS (from weak, in English), both charged W^{\pm} or the neutrons Z^{0} .

It has unspecific potential.

Charged weakons interfere in the β proton-neutron transformation reactions at the level of nucleus, such as,

With $s(W^{\pm}, Z^{\circ})=1$ spin.

With masses $m_0(W^{\pm})$ ~84 GeV (or protonic masses m_p), $m_0(Z^0)$ ~94 GeV. Discovered at CERN in 1983 (in January W^{\pm} , in June Z^0) by the team of Carlo Rubia and Simon Van der Meer (awarded with Nobel Prize in 1984).

1.2.3.2.4 GRAVITATIONAL INTERACTION

It occurs between the bodies with mass, being mediated by GRAVITON- Γ .

- With $s(\Gamma)=2$ spin.
- With zero rest mass $m_0(\Gamma)=0$.
- It moves with the light speed.
- Graviton is carried by the gravitational waves.
- Undetected yet.

The specific potential is written as:

$$V_G = -G\frac{M_1M_2}{r} \tag{64}$$

By unification of fundamental forces, respectively the first three interactions types of the Nature generate the so-called GUT (Grand Unification Theory) model, which extended to the fourth interaction- the Gravitational one, actually provides the weakest form the TOE (Theory of Everything) picture, with the schematically representation in Fig. 1.6.

Phenomenologically, the final unification which occurs at the so-called Planck scale era level, in Fig. 1.7 can be analytically explained in a direct manner, effectively considering the macro-micro cosmos unification, both at gravitational and quantum level, using the fundamental formulas of gravity, theory of relativity, along with the Planck quantification of energy:

$$E = hv = \frac{h}{t} \tag{65}$$

Quantum Nanosystems: Structure, Properties, and Interactions

$$ma = G \frac{mM}{r^2} \tag{66}$$

This way, one obtains the universal constant of gravity relationship

$$G = \frac{ar^2}{M} \tag{67}$$

which can be eventually equivalently written in "Planck manner" involving only universal constants (supposed unified or at least inter-exchangeable at the level of the grand unification of forces, particles and energies immediately after Big-Bang)

$$G = \frac{L_P c^2}{M_P} \tag{68}$$

where everything that is not an universal constant becomes a Planck quantity, specific to the birth of Universe!



FIGURE 1.6 Representation in relativistic space-time cones' paradigm (the so-called "Feynman diagrams") of fundamental interactions, quantized by specific particles which intermediate the typical elementary particles, see the text, superimposed to the scale of fundamental forces in relation with their reciprocal strength and the domain of distance where it is applicable (adaptation after Stierstadt K., Physik der Materie, VCH-Wiley, Weinheim, 1989, p. 42).



FIGURE 1.7 Unification paradigm of fundamental forces of Nature in relation with time, temperature and energy of dominant particles in the specific age along to the evolution of Universe; adapted after HyperPhysics 2010 (http://hyperphysics.phy-astr.gsu.edu/hbase/hph.html).

On the other side, using the Broglie's relation

$$p\lambda = h \tag{69}$$

rewritten at the Planck Universe level, a second working relation is obtained

$$(M_P c)L_P = h \tag{70}$$

which combined with the first from above Eq. (68), it firstly allows the elimination of Planck length, for example, by dividing the two relations, resulting in the Planck mass

$$M_P = \sqrt{\frac{ch}{G}} \cong 5 \cdot 10^{-8} [kg] \tag{71}$$

which further allows the length of early Universe (Planck) to be found

Quantum Nanosystems: Structure, Properties, and Interactions

$$L_P = \sqrt{\frac{Gh}{c^3}} \cong 4 \cdot 10^{-35} [m]$$
(72)

generating a set of cascade determinations, as the Planck time

$$t_P = \frac{L_P}{c} = \sqrt{\frac{Gh}{c^5}} \cong 10^{-43} [s]$$
(73)

driving the Planck energy calculation

$$E_P = \frac{h}{t_P} = \sqrt{\frac{hc^5}{G}} \cong 5 \cdot 10^9 [J] \cong 3 \cdot 10^{19} [GeV]$$
(74)

and implying the *Planck's temperature*

$$T_{P} = \frac{E_{P}}{k_{B}} = \sqrt{\frac{hc^{5}}{Gk_{b}^{2}}} \cong 3 \cdot 10^{32} [K]$$
(75)

while being accompanied by a colossal density of the early Planck Universe

$$\rho_P = \frac{M_P}{L_P^3} = \frac{c^5}{hG^2} \cong 10^{96} [kg / m^3]$$
(76)

This is how by unifying the quantum, gravitational and relativistic concepts one can obtain in fact a physical characterization of Big-Bang moment until the Planck horizon, by space-temporal parameters, in terms of mass, thermal and energetic expressions only, and by universal constants (Planck constant, Boltzmann constant, light speed in vacuum, universal gravity constant) as all of these would be unified in a single entity [31–70].

1.2.4 BLACK BODY RADIATION

For modeling photon radiation, the starting point is represented by the law of Bose-Einstein statistic

$$N_i = \frac{g_i}{\exp\left(\frac{\varepsilon_i - \mu}{k_B T}\right) - 1}$$
(77)

which it will be properly adapted, under the following peculiarities.

Nanouniverse Expanding Macrouniverse

Considering the fact that for photons, at equilibrium, the condition of constancy of the total number of particles $N \neq ct$ is not operating, wherefrom results the appropriate Lagrange multiplier cannot be applied, and therefore the associated chemical potential is zero

$$\mu = 0 \tag{78}$$

The degeneration of multiplicities can not be applied regarding the spin, but because there are two types of electromagnetic polarization (g = 2), the transition from *discrete* statistic to continuous one is done through the *small space* of phases, quantum normalized (in accordance with Heisenberg localization/ delocalization)

$$N_i \to dN = \frac{1}{\exp\left(\frac{\varepsilon}{k_B T}\right) - 1} \left(\frac{g}{a} d\gamma\right)$$
(79)

where, for the photon particles (with three degrees of freedom) we have

$$a = \left(2\pi\hbar\right)^3 = h^3 \tag{80}$$

with the elementary volume of phases

$$d\gamma = (dxdp_x)(dydp_y)(dzdp_z) = drdp = dV(4\pi p^2 dp)$$
(81)

rewritten by adapting the energy-momenta particle relationship for the photon

$$\varepsilon = c \cdot p \tag{82}$$

expressed as

$$d\gamma_p = 4\pi V \frac{\varepsilon^2}{c^2} \frac{d\varepsilon}{c}.$$
(83)

With this, the photon statistics becomes

$$dN = \frac{8\pi}{ac^3} V \frac{\varepsilon^2 d\varepsilon}{\exp\left(\frac{\varepsilon}{k_B T}\right) - 1}.$$
(84)

Based on these statistics, the total energy of photon radiation is obtained, by passing from the discrete definition to the continuous one

$$U = \sum_{i} \varepsilon_{i} N_{i} \to \int \varepsilon dN \tag{85}$$

and is successively calculated

$$U = \frac{8\pi}{ac^3} V \int_0^\infty \frac{\varepsilon^3 d\varepsilon}{\exp\left(\frac{\varepsilon}{k_B T}\right) - 1}$$

$$\stackrel{\varepsilon}{\stackrel{=}{=}} \overset{=}{\frac{8\pi V}{ac^3}} (k_B T)^4 \underbrace{\int_{0}^{\infty} \frac{x^3 dx}{\exp(x) - 1}}_{\pi^4/15}$$

$$=\frac{8\pi V}{ac^{3}} \left(k_{B}T\right)^{4} \frac{\pi^{4}}{15}$$
(86)

where the value of Riemann-zeta function has been used, under its third order form

$$\int_{0}^{\infty} \frac{x^{3} dx}{\exp(x) - 1} = \frac{\pi^{4}}{15}$$
(87)

If one considers the density of energy

$$u = \frac{U}{V} = \frac{8\pi^5 k_B^4}{15h^3 c^3} T^4$$
(88)

this can be used to define the so-called radiance or energy flux density or radiant flux (energy emitted by a blackbody per unit area per unit time, or the radiant power per unit area)

$$L = \int dL = \frac{P}{A} = \frac{U}{A \cdot t} = \frac{x}{t} \frac{U}{A \cdot x} = \frac{c}{4}u$$
(89)

which further takes the expression of the so-called Stefan-Boltzmann law

$$L = \sigma T^4 \tag{90}$$

where the Stefan constant has been introduced

$$\sigma = \frac{2\pi^5 k_B^4}{15h^3 c^3} = 5.670400 \times 10^{-8} [J \cdot s^{-1} \cdot m^{-2} \cdot K^{-4}]$$
(91)



FIGURE 1.8 The geometrical configuration, which express the photonic radiance; adapted from HyperPhysics 2010 (http://hyperphysics.phy-astr.gsu.edu/Hbase/hframe. html).

Note that the factor $\frac{1}{4}$, from the radiation definition (89), comes from the geometrically condition of integration upon the values of possible radiation angles, toward a given source, as shown in Fig. 1.8:

$$\Delta U = L \cdot t \cdot \Delta A$$
$$= \underbrace{2}_{\pm x} \frac{\Delta L}{\cos \theta} \cdot \frac{\Delta t}{\cos \theta} \cdot \Delta A$$
$$= 2 \underbrace{\frac{1}{\cos^2 \theta}}{\frac{\Delta x}{c}} \cdot \Delta L \Delta A \tag{92}$$

wherefrom results the customary expression

$$L = \int_{\theta} \Delta L d\theta = \frac{\Delta U}{\Delta V} \frac{c}{2} \underbrace{\frac{1}{2} \frac{\int_{-\pi/2}^{\pi/2} \cos^2 \theta d\theta}}_{1/2} = \frac{c}{4} u$$
(93)

- \

Moving forward, if we rewrite the density of total radiant energy in quantification of Planck radiation $\varepsilon = hv$, then, the integral is formed

$$u = \frac{U}{V} = \frac{1}{h^3} \int_0^\infty \frac{8\pi}{c^3} \frac{(h\nu)^3 d(h\nu)}{\exp\left(\frac{h\nu}{k_BT}\right) - 1}$$

$$= \int_{0}^{\infty} \frac{8\pi h}{c^{3}} \frac{v^{3} dv}{\exp\left(\frac{hv}{k_{B}T}\right) - 1}$$
$$\equiv \int_{0}^{\infty} \rho(v, T) dv$$

wherefrom the energy spectral density (in frequency) is identified

$$\rho(v,T) = \frac{8\pi h}{c^3} \frac{v^3}{\exp\left(\frac{hv}{k_B T}\right) - 1}$$
(95)

(94)

which corresponds to the Planck formula (distribution) of the blackbody radiation! Note that Planck used his formula under the spectral intensity form as the quantity of emitted energy by a blackbody at temperature T per unit area, per unit time, per unit solid angle, in the (v, v + dv) interval – that is, the unit of frequency:

$$I(v,T) = \frac{1}{\Omega} \frac{1}{t} \frac{1}{A} \frac{dU}{dv}$$
$$= \frac{1}{4\pi} \frac{1}{t} \frac{V}{\frac{A}{\Delta}} \frac{8\pi h}{c^3} \frac{v^3}{\exp\left(\frac{hv}{k_0T}\right) - 1}$$

$$=\frac{2hv^3}{c^2}\frac{1}{\exp\left(\frac{hv}{k_BT}\right)-1}$$

28

Nanouniverse Expanding Macrouniverse

$$=\frac{c}{4\pi}\rho(v,T)\tag{96}$$

Another important quantity related to the energy density is referring to the photon radiation pressure, phenomenological deduced from the general relations

$$P_{\gamma} = \frac{Force}{Area} = \frac{1}{A} \frac{dp}{dt} \stackrel{\varepsilon = c \cdot p}{=} \frac{1}{c} \frac{1}{\underline{A}} \frac{d\varepsilon}{dt} \propto \frac{1}{c} (c \cdot u) = u$$
(97)

and which, by taking into consideration the statistical geometric conditions, in the framework of equipartition of the three considered coordinate, we will have the working formula for the radiation pressure

$$P_{\gamma} = \frac{1}{3}u = \frac{1}{3}\sigma^* T^4$$
(98)

It is worth noting that in astrophysics, there is often used the alternative form of the Stefan-Boltzmann law, written at the energy density level

$$u = \sigma^* T^4 \tag{99}$$

with the new Stefan constant (Stefan-star)

$$\sigma^* = \frac{4\sigma}{c} = \frac{8\pi^5 k_B^4}{15h^3 c^3} = 7.565767 \times 10^{-16} [J \cdot m^{-3} \cdot K^{-4}]$$

These are the theoretical premises that will allow us to characterize the various bodies of the universe (the Sun, the Earth, the Stars and even the Cosmos as an ensemble) based on electromagnetic radiation emitted or stored by them [71–84].

1.3 FERMI-WEINBERG TYPE ESTIMATIONS OF UNIVERSE'S DARK MATTER AND ENERGY

1.3.1 ELEMENTARY PARTICLES IN UNIVERSE AND PHYSICAL CONSEQUENCES

One starts with the Table 1.2, which resumes the physical properties of elementary particles; it can be observed that the photons and the neutrinos are the only particles assumed to have null rest mass, implicitly with the possibility of creation (from quantum or subquantum vacuum) at any nonnull