Numerical physics
Specific problems and applications

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Abstract. In this period of very fast increasing of the technical possibilities of computers, as well as of the number of published works, the Numerical Physics most provide: a) some *accurate criteria intended to the evaluation of the compatibility of a theoretical model relative to the experimental results*, b) *computing algorithms* which ensure: (i) a *satisfactory accuracy*, avoiding the instability and non-convergence phenomena and limiting the dispersion-distortion phenomena, (ii) a *minimal duration of calculations* (numerical simulations). The part of Physics which can solve these problems corresponds to the chapter 0260 (Numerical Approximation and Analysis) in the international classification of Physics Abstracts; one finds so that the Numerical Physics is a kind of "projection" in Physics of the field 65 (Numerical Analysis) of Mathematical Reviews.

The field of Numerical Physics has the support of Mathematics and of Theoretical Physics, providing the necessary algorithms for the computing codes used by the Computational Physics. Surely, the results of numerical computations have *many applications, both in the field of Theoretical Physics and in different domains of Applied (Technical) Physics.* Taking into account that the validity domain of the different Physics theoretical models corresponds to some numerical values of the similitude criteria, one finds that *the Numerical Physics is also very important* for the classification of these domains and, *for the Physics teaching (in frame of Technical Universities, especially)*, consequently.

I. Introduction

§1.1. *The structures of the modern Mathematics and Physics, respectively; the specific tasks of the Computational Physics and of the Numerical Physics*

The next Diagram 1 presents the structures of modern Mathematics (according to Mathematical Reviews Contents) and Physics (according to Physics Abstracts), respectively. One finds the existence of a certain "superposition" of these basic sciences; e.g., the Physics is "represented" in frame of Mathematics by the domains: Mechanics of particles and systems (domain 70), Mechanics of solids (73), Optics, electromagnetic theory (78), Classical thermodynamics, heat transfer (80), Quantum theory (81), Statistical mechanics (82), Relativity and gravitational theory (83), Astronomy and astrophysics (85), Geophysics (86), while the Mathematics is present in Physics mainly due to the domain Mathematical Methods in Physics (0200), with the sub-domains referring to: Algebra, set theory, and graph theory (field 0210), Group theory (0220), Function theory, analysis (0230), Geometry, differential geometry, and

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topology (0240), Probability theory, stochastic processes, and statistics (0250), *Numerical Approximation and Analysis* (0260), Computational techniques (0270) and Other topics in mathematical methods in Physics (0280).

Diagram 1

MAIN PRESENT DOMAINS OF MATHEMATICS AND PHYSICS
according to:

MATHEMATICAL REVIEWS CONTENTS

00: General
01: History and biography
03: Mathematical logic and foundations
04: Set theory
05: Combinatorics
06: Order, lattices, ordered algebraic systems
08: General algebraic systems
11: Number theory
12: Field theory and polynomials
13: Commutative rings and algebras
14: Algebraic geometry
15: Linear and multilinear algebra; matrix theory
16: Associative rings and algebras
17: Nonassociative rings and algebras
18: Cathegory theory homological algebra
19: K-theory
20: Group theory and generalizations
22: Topological groups, Lie groups
26: Real functions
28: Measure and integration
30: Functions of complex variable
31: Potential theory
32: Several complex variables and analytical spaces
33: Special functions
34: Ordinary differential equations
35: Partial differential equations
39: Finite differences and functional equations
40: Sequences, series, summability
41: Approximations and expansions
42: Fourier analysis
43: Abstract harmonic analysis
44: Integral transforms, operational calculus
45: Integral equations
46: Functional analysis
47: Operator theory
49: Calculus of variations and optimal control; optimization
51: Geometry
52: Convex and discrete geometry
53: Differential geometry
54: General topology
55: Algebraic topology
57: Manifolds and cell complexes
58: Global analysis, analysis in manifolds
60: Probability theory and stochastic processes
62: Statistics
65: NUMERICAL ANALYSIS
68: Computer science
70: Mechanics of particles and systems
73: Mechanics of solids
78: Optics, electromagnetic theory
80: Classical thermodynamics, heat transfer
81: Quantum theory
82: Statistical mechanics
83: Relativity and gravitational theory
85: Astronomy and astrophysics
86: Geophysics
90: Economics, operations research, programming, games
92: Biology and natural sciences, behavioral sciences
93: Systems theory, control
94: Information and communication circuits

PHYSICS ABSTRACTS

0000: GENERAL
0100: Communication, Education, History, and Philosophy
0200: Mathematical Methods in Physics
0210: Algebra, set theory, and graph theory
0220: Group theory
0230: Function theory; analysis
0240: Geometry, differential geometry, and topology
0250: Probability theory, stochastic processes, and statistics
0260: Numerical Approximation and Analysis
(NUMERICAL PHYSICS)
0270: Computational techniques
0280: Other topics in mathematical methods in physics
1000: The Physics of elementary Particles and Fields
2000: Nuclear Physics
3000: Atomic and Molecular Physics
4000: Fundamental Areas of Phenomenology
5000: Fluids, Plasmas and Electric Discharges
6000: Condensed Matter; Structure, Mechanical and Thermal Properties
7000: ibid.; Electronic Structure, Electrical, Magnetic and Optical Properties
8000: Cross-Disciplinary Physics and Related Areas of Science and Technology
9000: Geophysics,Astronomy and Astrophysics

One finds so that the Numerical Physics acts mainly in frame of the sub-domain Numerical Approximation and Analysis (0260), being a true "projection" in Physics of the domain 58: "Numerical Analysis" of Mathematics. On the other hand, the Numerical Physics is a part of the Computational Physics, namely that part which elaborates the (physical) algorithms of the studied problems, while the Computational Physics needs and involves also many elements concerning the used Computational techniques. The position of the Numerical Physics relative to Mathematics and in frame of Physics and of the Computational Physics, resp. is presented by Diagram 2.

Unlike the considerable number of the existing textbooks of Computational Physics (see e.g. the references [1]-[7], as well as of the books of Numerical Methods for Physics [8]), we did not yet meet similar textbooks of Numerical Physics, despite of the considerable interest corresponding to its specific problems and applications. The study of the structure of **the Computational Physics textbooks** points out (Diagram 3), that they **start always from the mathematical knowledge necessary for the basic calculations in Physics**, the typical applications (in many important Physics problems) following the mathematical knowledge.

Taking into account that **the Numerical Physics starts always from some numerical problems specific to Physics**, a short previous analysis of the main conceptual differences between Mathematics and Physics is absolutely necessary.

Diagram 2

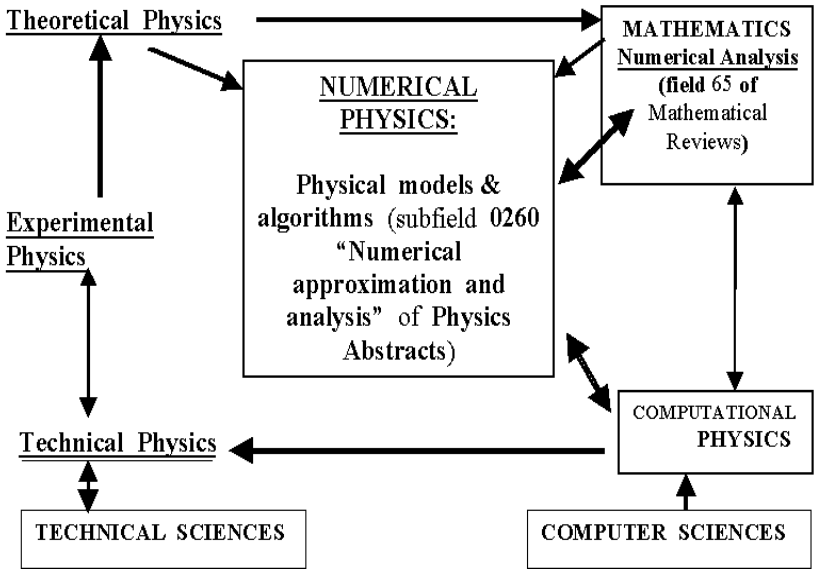


Diagram 3a

The content of the Computational Physics textbook: Steven E. Koonin "Computational Physics", Addison-Wesley Publishing Company, 1986

Chapter 1: Basic Mathematical Operations (§1.1. Numerical differentiation, §1.2. Numerical quadrature, §1.3. Finding roots, §1.4. Semiclassical quantization of molecular vibrations, Project I: Scattering by a central potential) ..... 22 pages

Chapter 2: Ordinary Differential Equations (§2.1. Simple methods, §2.2. Multistep and implicit methods, §2.3. Runge-Kutta methods, §2.4. Stability, §2.5. Order and chaos in 2D motion, Project II: The structure of white dwarf stars (II.1. The equations of equilibrium, II.2. The equation of state, II.3. Scaling the equations, II.4. Solving the equations)) ..... 26 pages

Chapter 3: Boundary Value and Eigenvalue Problems (§3.1. The Numerov algorithm, §3.2. Direct integration of boundary value problems, §3.3. Green's function solution of boundary value problems, §3.4. Eigenvalues of the wave equation, §3.5. Stationary solutions of the 1D Schrödinger equation, Project III: Atomic structure in the Hartree-Fock approximation (III.1. Basis of the Hartree-Fock approximation, III.2. The two-electron problem, III.3. Many-electrons systems, III.4. Solving the equations)) ..... 28 pages

Chapter 4: Special Functions and Gaussian Quadrature (§4.1. Special functions, §4.2. Gaussian quadratures, §4.3. Born and eikonal approximations to quantum scattering, Project IV: Partial wave solution of quantum scattering (IV.1. Partial wave decomposition of the wavefunction, IV.2. Finding the phase shifts, IV.3. Solving the equations)) 24 pages

Chapter 5: Matrix Operations (§5.1. Matrix inversion, §5.2. Eigen-values of a tri-diagonal matrix, §5.3. Reduction to tri-diagonal form, §5.4. Determining nuclear charge densities, Project V: A schematic shell model (V.1. Definition of the model, V.2. The exact eigenstates, V.3. Approximate eigenstates, V.4. Solving the model)) ..... 36 pages

Chapter 6: Elliptic Partial Differential Equations (§6.1. Discretization and the variational principle, §6.2. An iterative method for boundary value problem, §6.3. More on discretization, §6.4. Elliptic equations in 2D, Project VI: Steady-state hydrodynamics in 2D (VI.1. The equations and their discretization, VI.2. Boundary conditions, VI.3. Solving the equations)) ..... 24 pages

Chapter 7: Parabolic Partial Differential Equations (§7.1. Naive discretization and instabilities, §7.2. Implicite schemes and the inversion of tri-diagonal matrices, §7.3. Diffusion and boundary problems in 2D, §7.4. Iterative methods for eigenvalue problems, §7.5. The time-dependent Schrödinger equation, Project VII: Self-organization in chemical reactions (VII.1. Description of the model, VII.2. Linear stability analysis, VII.3. Numerical solution of the model)) ..... 24 pages

Chapter 8: Monte Carlo methods (§8.1. The basic Monte Carlo strategy, §8.2. Generating random variables with a specified distribution, §8.3. The algorithm of Metropolis et al., §8.4. The Ising model in 2D, Project VIII: Quantum Monte Carlo for the H_2 molecule (VIII.1. Statement of the problem, VIII.2. Variational Monte Carlo and the trial wavefunction, VIII.3. Monte Carlo evaluation of the exact energy, VIII.4. Solving the problem) ..... 32 pages

Appendix A: Synopsis of the BASIC language ..... 10 pages

Appendix B: Programs for the Examples (B1. Finding the semiclassical approximations to the bound state energies of the Lennard-Jones potential for the value of $\gamma = \sqrt{2ma^2V_o/\hbar^2}$ input, B2. Integration of trajectories in the Hénon-Heiles potential and obtainment of the corresponding surfaces of section, B3. Obtainment of the stationary states of the 1D-Schrödinger equation for a particle in a potential normalized so that its maximum and minimum values are +1 and –1, resp., B4. Calculation of the Born and eikonal scattering amplitudes and cross-sections for an electron incident on a square-well, Gaussian-well, or Lenz-Jensen potential, as described in the text, B5. Fitting of the electron-nucleus elastic scattering cross sections to determine the nuclear charge density using the method described in the text, B6. Solving the Laplaçe's equation in 2D on a uniform rectangular lattice by Gauss-Seidel iteration, B7. Solving the time-dependent Schrödinger equation for a particle moving in 1D, B8. Simulation of the 2D Ising model using the algorithm of Metropolis et al.) . 110 pages

A similar structure, but involving also some elements concerning the Errors and Uncertainties in Computations (Blunders, Random errors, Approximation Errors and Roundoff Errors) and those intervening in Algorithms, as well as some elements concerning the Computation Techniques, has the recent Computational Physics book of R.H.Landau and M.J.Páez [6]. The titles of the chapters involved by this book are indicated in the last part of Diagram 3b.

Diagram 3b

The content (titles of Chapters) of the book of R.H.Landau, M.J.Páez Mejía "Computational Physics. Problem Solving with Computers", John Wiley and Sons, Inc., New York-Chichester-Weinheim-Brisbane-Singapore-Toronto, 1997

Part I. Generalities (1. Introduction, 6 pages, 2. Computing Software Basics, 22 pages, 3. Errors and Uncertainties in Computations, 16 pages, 4. Integration, 19 pages)

Part II. Applications (5. Data Fitting, 20 pages, 6. Deterministic Randomness, 10 pages, 7. Monte Carlo Applications, 16 pages, 8. Differentiation, 8 pages, 9. Differential Equations and Oscillations, 14 pages, 10. Quantum Eigenvalues; Zero-Finding and Matching, 12 pages, 11. Anharmonic Oscillations, 8 pages, 12. Fourier Analysis of Nonlinear Oscillations, 20 pages, 13. Unusual Dynamics of Nonlinear Systems, 10 pages, 14. Differential Chaos in Phase Space, 16 pages)

Part III. Applications: High Performance Computing (15. Matrix Computing and Subroutine Libraries, 34 pages, 16. Bound States in Momentum Space, 8 pages, 17. Quantum Scattering via Integral Eqauations, 10 pages, 18. Computing Hardware Basic: Memory and CPU, 14 pages, 19. High-Performance Computing: Profiling and Tuning, 12 pages, 20. Parallel Computing and PVM, 8 pages, 21.

Object-Oriented Programming: Kinematics, 14 pages, 22. Thermodynamic Simulations, 12 pages, 23. Functional Integration on Quantum Paths, 14 pages, 24. Fractals, 20 pages)

Part IV. Partial Differential Equations (25. Electrostatic Potentials, 12 pages, 26. Heat Flow, 10 pages, 27. Waves on a String, 14 pages, 28. Solitons, the DdeV Equation, 10 pages, 29. Sine-Gordon Solitons, 10 pages, 30. Confined Electronic Wave Packets, 10 pages)

Appendices: A. Analogous Elements in Fortran and C, 2 pages, B. Programs on Floppy Diskette, 6 pages, C. Listing of C Programs, 44 pages, D. Listing of Fortran Programs, 40 pages, E. Typical Project Assignments, 2 pages, Glossary – 2 pages and References – 5 pages.

§1.2. *Short analysis of the main conceptual differences between Mathematics and Physics*

While: a) *the Physics of macroscopic systems* (represented mainly by Mechanics) *presents a deterministic character*, which allowed its very quick axiomatization by Ernst Mach et al., b) *the phenomena at the mesoscopic level* (dimensions of the magnitude order of 1 μm) of the grains from metals, alloys, rocks etc. *present both hysteretic and considerably strong nonlinear behaviors*, that does difficult (often impossible) the deterministic descriptions, and: c) *the phenomena at the microscopic (atomic) level have a net quantum (probabilistic) character.*

That is why – unlike to the usual mathematical concepts – an absolutely exact (from the view point of the classical determinism) description of the physical systems is usually impossible.

A first direct consequence of this experimental finding refers to the problem of uniqueness parameters. This consequence represents *a first important difference between the mathematical and physical concepts, resp.*: *While the number of uniqueness parameters of a mathematical problem is fixed* (e.g. 3 for an arbitrary triangle: the lengths of the triangle sides, or the lengths of 2 sides and the angle between these sides etc.), *the number of uniqueness parameters of a physical system depends on the required accuracy of the obtained description.* E.g., while the thermodynamic state (mass density, volume density of the internal energy, etc) of the air is mainly described by 2 uniqueness parameters (the air temperature and pressure), an improvement of the description accuracy needs to take into consideration an additional (a third one) uniqueness parameter: the air humidity, another increase of the description accuracy requires a fourth uniqueness parameter: the content of carbon dioxide, etc.

The second important difference between the mathematical and physical concepts refers to the definition of a well-possessed problem. While in Mathematics a such problem corresponds usually to a system of compatible and non-redundant equations, whose number is equal to that of unknowns, a well-possessed Physics problem needs a system of (slightly) incompatible (and non-redundant) equations, whose number must be considerably larger than that of unknowns.

The above definition of a well-possessed Physics problem reflects already the existence of fluctuations (due to the microscopic structure) and even the presence of

some hysteretic behaviors (due to the mesoscopic structure) of the studied physical system. It appears here *a third important difference between the mathematical and physical concepts:* while in Mathematics the obtained results are exact (therefore their confidence level is the maximum one: $L = 1$) and they correspond to a real obtained information ($\Im$¿0), the Physics results are connected always with some specific confidence levels ($L < 1$) and sometimes the obtained apparent information could correspond really to a misinformation ($\Im$¡0).

Finally, we consider that *a fourth* (and last) *important difference between the mathematical and physical concepts* refers to the method of incomplete induction. While in Mathematics, the incomplete induction is only the first step of the rigorous (and exclusively accepted) method of the complete induction, in Physics the method of the incomplete induction is accepted and represents even one of the main Physics methods (also of the Numerical Physics) [1].

§1.3. Main Functions of the Numerical Physics

Taking into account the existing differences between the mathematical and physical concepts, the above presented main possibilities of the Computational Physics, as well as the relations of the Numerical Physics with Mathematics and the Computational Physics, this work has found that the Numerical Physics represents:

a) *the Physics version of the theory of field 0260 "Numerical Approximation and Analysis", as a componentof the domain 0200 "Mathematical Methods in Physics" of the Physics Abstracts Classification* (as it can be found from Diagram 1, the Numerical Physics represents the end located in Physics of the "bridge" which connects the Mathematics and Physics),

b) *the Theory of Physics Models* (as it was shown above, the Numerical Physics represents also a "projection" of the field 65 of Mathematics in Physics; taking into account that the main purpose and application of the Numerical Analysis is the study of the general (abstract) models, it results that **one of the main goals of the Numerical Physics consists in the study of physical models**),

c) *a general method of Physics intended to the obtainment and to the study of the meaning of physical numbers* (as the experimental Physics uses mainly the experimental methods for the Physics study, as the theoretical Physics highlights the concepts, basic equations, principles and other theoretical elements to study the Physics, and the technical Physics studies mainly the physical instruments and devices and their applications, the Numerical Physics highlights the physical numbers, studying and underlying their specific meanings and uses; because **this function is the most important one**, the Numerical Physics represents the physical findings expressed and multiply checked by numbers),

d) *the Proto-Mathematics* (as it can be found from Diagram 1, the Numerical

[1] For this reason, the set of Physics principles is not equivalent to the experimental results which have generated them. This non-equivalence allows to the theoretical Physics, which obtains rigorous deductions (but starting from the Physics principles, obtained by means of the incomplete induction method!), to find some extremely important new results (e.g. concerning the population inversion, the nuclear energy etc.) many years before their experimental discovery.

Physics (and its associated field 0260) represents a true "pump", which sends permanently towards Mathematics new algebraic structures specific to certain Physics domains (see the domains 70...86 of the Mathematical Reviews Contents from Diagram 1); it results that the Numerical Physics could be considered as a previous stage of many domains of Mathematics, i.e. as a true Proto-Mathematics).

Taking into account the considerable number of different functions of the Numerical Physics, it is easy to understand its important and various scientific, technical and didactic applications.

II. Basic notions of Numerical Physics

Taking into account the central role of correlations for the study of the nature sciences[2], it is necessary to classify the basic notions of Physics (as the main nature science, the others being the Physical Chemistry, the Biophysics, the Physical Electronics, the Astrophysics etc) as: (i) *pre-correlational notions,* (ii) *notions specific to correlations*, (iii) *post-correlational notions.*

§2.1. *Definitions of the main pre-correlational notions*

Because some of the pre-correlational notions are defined starting from notions of Mathematical Statistics, these parameters can be classified as:

a) *Pre-correlational notions, whose definitions do not need statistical notions:*

The main such notions are: (i) *the physical property*, (ii) *the physical quantity*, (iii) *the physical measure*, (iv) *the physical units and magnitudes (*relative to a certain physical measure), resp., (v) *the physical amount*, (vi) *the physical parameter*,

b) *Notions of Mathematical Statistics, intervening in definitions of some pre-correlational notions:*

(i) the non-conditioned and the conditioned probabilities, (ii) the density of probability in a continuous N-dimensional space, (iii) some particular discrete (Bernoulli, Poisson (of rare events) etc) and continuous (the normal N-dimensional distribution, with its particular 2D- and 1D- (Gauss) cases) probability distributions, (iv) the principles and the specific features of the main statistical tests used in Physics.

c) *Pre-correlational notions defined by means of some statistical notions:*

The main such notions are: (i) *the true* (most probable) *value* a_{Xi}*of a physical parameter* X_i, (ii) *the physical errors* $\varepsilon_{Xi} \equiv \varepsilon(X_i) = x_i - -a_{Xi}$ (where $x_i$is *the measured individual value*)*, their classification and their associated notions,* mainly: (iii) *the covariance:* $Cov(X,Y) =< \varepsilon(X_i) \cdot \varepsilon(Y_i) >$ and: (iv) *the variance (dispersion):* $D(X) \equiv Cov(X,X) =< \varepsilon^2(X_i) >$, (v) *the confidence domains and levels*, resp.

The definitions of these notions are presented by works [11], p. and [12], p.484-486.

§2.2. *Definitions of the main notions specific to correlations*

The most important correlational notions are those referring to the: a) *uniqueness parameters* u_k (k*=1,2,...*m), b) *the parameters of material (system)* p_j (j*=1,2...*n) *and their zero-order approximations*, c) *tested* (measurable) *parameters* t_i (i*=1,2,...*N),

[2]This opinion belongs to A. Einstein [9], page 67, R. Feynman [10], vol.1, page 36 etc.

whose measured (experimental) values $t_{\exp .i}$ can be also evaluated (calculated) theoretically, starting from the values of the uniqueness parameters and those of the material (system) parameters: $t_{calc.i} = f_i(u_k, p_j)$, d) *the weights* W_i *(i=1,2,...N) associated to the experimental values of the test(ed) parameters, usually chosen as:* $W_i = \frac{C}{D(t_i)}$, where $C$is a conveniently chosen constant, e) *principle of the minimum square deviations:* the most probable values of the material (system) parameters p_j are those corresponding to the minimum of the sum of weighted squares: $S = \sum_{i=1}^{N} W_i \left(t_{calc.i} - t_{\exp .i}\right)^2$, e) *the algorithm of the gradient* (Jacobi's) *method and its involved main notions.* The definitions and descriptions of these notions are discussed by works [11], p. and [12], p.486-488.

§2.3. *Definitions of the main post-correlational notions*

The most important post-correlational notions refer to: a) *the physical correlations and their classification* (as legal correlations or semiempirical ones), b) *the classification of the legal correlations* (as physical theorems and laws, respectively), c) *the incomplete induction method of Physics*, d) *the classification of the main results of the Physics incomplete induction method, starting from the Physics legal correlations* (as Physics postulates and principles, respectively), e) *the classification of physical constants* (as material parameters, universal or fundamental constants, respectively), f) *the definitions of the fundamental physical quantities and units, respectively,* g) *the definition of the rationalization coefficients*, h) *the definitions of the main systems of physical quantities and units* (mainly of the international system SI, of the electrostatic $CGS\varepsilon_o$, magnetostatic $CGS\mu_o$ and Gauss ($CGS\varepsilon_o\mu_o$) systems, respectively), i) *the definition of the physical dimension and its applications* (the dimensional analysis), j) *the definitions of the uniqueness parameters and of the corresponding similitude indices*, k) *the definitions of the similar states* (or processes) *and of the similitude numbers* (criteria), l) *the theorems of the theory of physical similitude and their theoretical* (classification of the validity domains of the main Physics theoretical models) *and technical application* (the theory of the laboratory experimental models).

III. Specific problems of the Numerical Physics

§3.1. *The Choice of the Uniqueness Parameters*

From the definition of the uniqueness parameters, it results that the physical descriptions start from these parameters, the main method used to ensure accurate descriptions being that of the gradient (Jacobi's) method. Taking into account that some inaccurate zero -order approximations of the uniqueness parameters could lead to wrong (non-physical) results, it is necessary to prefer (as uniqueness parameters) the parameters which can be measured directly, and with the highest accuracy, preferably.

For this finding is valid (from the point of view of physicists) even for the some problems of Mathematics, we will present firstly the example of the choice of the uniqueness parameters for the point groups of the operations of rotations and mirroring in the 3D-space.

a) *The uniqueness parameters of the 3D-rotation & mirroring point groups*

The choice of the uniqueness parameters of the 3D-rotation and mirroring point groups by means of the: (i) *Euler's angles*, (ii) *Cayley-Klein's parameters*, is well known [13]. Unfortunately, it is rather difficult to find – starting from the Euler's angles or the Cayley-Klein's parameters – the specific parameters of each point operation: the unit vector of the rotation axis (or of the normal on the mirroring plane) and the angle of rotation. That is why the choices of uniqueness parameters for the point groups, done by the classical Mathematics, are unsatisfactory from the point of view of physicists. For this reason, we will present here an alternative choice of the uniqueness parameters of the 3D point groups, whose chosen uniqueness parameters:

$$s = \det T \ , \qquad \bar{q} = \sin\left[\frac{\varphi}{2} + (s-1)\frac{\pi}{4}\right] \bar{1}_a, \tag{3.1.1}$$

are directly connected to the indicated parameters of Physics interest: the geometrical transformation matrix T, the rotation angle ϕ and the unit vector of the rotation axis (or mirroring plane, resp.) $\mathbf{1}_a$. In this case, one finds that the successive accomplishment of the point operations $P_1(\mathbf{q}_1,\, s_1)$ and – in following – $P_2(\mathbf{q}_2,\, s_2)$ is equivalent to a point operation whose parameters $\mathbf{q}$, s are given by the identity:

$$\hat{P}_2(\bar{q}_2, s_2) \cdot \hat{P}_1(\bar{q}_1, s_1) = \hat{P}\left[s_{12}\left(\tilde{q}_2\bar{q}_1 + \tilde{q}_1\bar{q}_2 - \bar{q}_1 \times \bar{q}_2\right), s_1 s_2\right] \ , \tag{3.1.2}$$

where *the norm of the dual of the vector* $\mathbf{q}$ and s_{12} are:

$$\tilde{q} = \left|\sqrt{1-q^2}\right| \ , \qquad s_{12} = sign\left(\tilde{q}_1\tilde{q}_2 - \bar{q}_1\bar{q}_2\right). \tag{3.1.3}$$

Similarly, one finds [13] that the above presented uniqueness parameters (3.1) allow direct expressions for: (i) the product of 3 point operations, (ii) the conjugate of a point operation relative to another point operation, (iii) the inverse of a point operation a.s.o., answering so to all usual requirements in Physics. Of course, the above defined uniqueness parameters can be correlated with the Euler's angles by means of relations:

$$\begin{array}{ll} q_x & = \sigma \cdot \sin\frac{\beta}{2} \cdot \cos\frac{\gamma-\alpha}{2} \\ q_y & = \sigma \cdot \sin\frac{\beta}{2} \cdot \sin\frac{\gamma-\alpha}{2} \\ q_z & = \sigma \cdot \cos\frac{\beta}{2} \cdot \sin\frac{\gamma+\alpha}{2} \ , \end{array} \tag{3.1.4}$$

[where $\sigma = s_{123}$ for: $\bar{q}_1 = \bar{q}(\bar{1}_z, \alpha, s_\alpha)$, $\bar{q}_2 = \bar{q}(\bar{1}_x, \beta, s_\beta)$, $\bar{q}_3 = \bar{q}(\bar{1}_z, \gamma, s_\gamma)$] and with the Cayley-Klein parameters by means of the expressions:

$$a = \sigma\left(\tilde{q} + i \cdot q_z\right) \ , b = \sigma\left(q_x + i \cdot q_y\right) \qquad \left(i = \sqrt{-1}\right) \ . \tag{3.1.5}$$

b) *Choice of the Uniqueness Parameters in the Problem of Thermally Stimulated Depolarization Currents (TSDC).*

The temperature dependence of the thermally stimulated depolarization currents (see Fig.1) is described by the classical equation [15]:

$$I(T) = \frac{Q_o}{\tau_o} \exp\left[-\frac{W}{kT} - \frac{T}{b\tau_o} E_2\left(\frac{W}{kT}\right)\right]. \tag{3.1.6}$$

One finds easily that while the uniqueness parameter b is given by the experimental time dependence of the temperature: $b=dT/dt$, the evaluation of other classical TSDC uniqueness parameters (the electrical charge Q_o under the peak of the $I_{TSDC}=f(t(T))$ plot, as well as of the relaxation time τ_o) is very difficult. Taking into account: (i) the particular importance of the choice of the zero-order approximations of the uniqueness parameters for certain numerical methods (e.g. for the gradient method, see the corresponding Section), and: (ii) the real difficulty to find sufficiently accurate zero-order approximations of some parameters (as Q_o and τ_o) which are not measured directly, a choice of some uniqueness parameters directly related to the experimentally measured parameters is really useful. That is why we proposed [16] to substitute the indirect valuable uniqueness parameters Q_o and τ_o by means of the maximum TSDC current I_m and the temperature T_m corresponding to this current (see Fig. 3.1):

$$\ln I(T) = \ln I_m + \frac{W}{k}\left(\frac{1}{T_m} - \frac{1}{T}\right)\left[T_m E_2(x_m) - T \cdot E_2(x)\right], \tag{3.1.7}$$

where $E_2(x)$is a function related to the "exponent integral" function $Ei(-x)$:

$$E_2(x) = \int_1^\infty e^{-x\cdot t} \cdot t^{-2} dt = e^{-x} - x\left(-Ei(-x)\right) \ , \tag{3.1.8}$$

and: $x= W/(kT)$ and: $x_m=W/(kT_m)$.

The accomplished study [16a-c] pointed out that the choice of some experimentally measured parameters as uniqueness parameters (I_m and T_m) allows both the accurate determination of the activation energy W and the accurate description of the temperature (time) dependence of the TSDC currents.

§3.2. *Knowledge and Use of Effective Parameters*

As it is well known, the physical models used to describe some physical states or phenomena cannot be absolutely exact. That is why the improvement of the measurement accuracy imposes new (more complex) physical models, which generalize the previous (more elementary) ones. The parameters of the simpler models which allow the description of some features of the studied complex physical system by means of these elementary models are named *effective parameters*. Of course, this definition is valid also for the numerical values obtained for some physical parameters by different experimental methods (e.g. the neutron diffraction *effective cross-section*

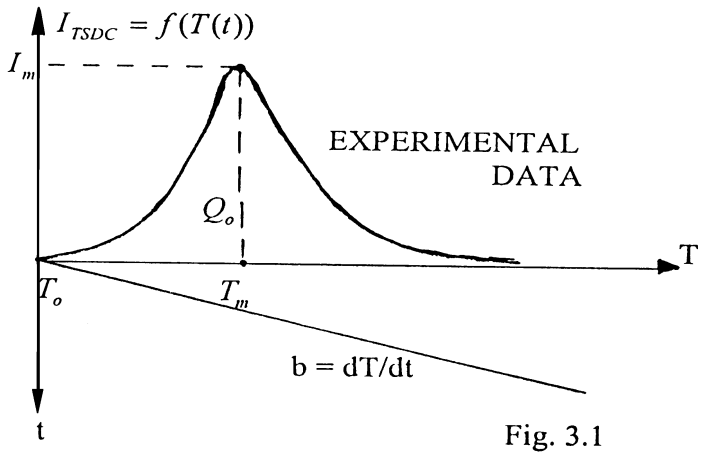


Fig. 3.1

refers to the cross-section of certain atomic nuclei, measured by means of the neutron diffraction).

An elementary example of effective parameters corresponds to the case of the power dissipated by a resistance under an alternating current. It is well known that this (average, usually named *active*) power is given by the expression:

$$P_a = \frac{1}{T}\int_0^T RI_o^2 \cos^2(\omega t + \varphi)\, dt = RI_o^2 \int_0^T \frac{1 - \cos 2(\omega t + \varphi)}{2T} dt = \frac{RI_o^2}{2} = RI_{eff}^2 \ ,$$

where: $I_{eff} = \frac{I_o}{\sqrt{2}} \cong 0.7071\ I_o$ is the so-called *effective current* (being related to the so-called *effective voltage* on the considered resistance by means of the relation: $U_{eff} = RI_{eff}$. One finds that *a direct current* I_{eff} dissipates, in the same duration, the same heat in the considered resistance as the alternating current of amplitude I_o.

Such effective parameters are met particularly for alternating fields, of arbitrary nature. So, we will present in following some examples of effective parameters associated to the: a) physical models intended to the description of the sound propagation through attenuative elastic media, b) electrical measurements in alternating currents of some electrical circuits involving hysteretic (nonlinear) components, c) intramolecular interactions and structures, taking into account the complex (involving oscillations of the atomic nuclei and other) intramolecular "motions".

The knowledge and proper use of the effective parameters allows: (i) to simplify the description of some (complex) physical systems, (ii) to obtain accurate numerical simulations of some rather intricate physical phenomena (for example of the multiple reflected and transmitted ultrasonic beams in composite materials) even for media with dispersive and nonlinear (hysteretic, inclusively) properties, (iii) to avoid the

appearance of some numerical heterogeneity by the introduction in the same semi-empirical relations of the values of some effective parameters of different physical nature.

a) *Effective Parameters Specific to the Description of Sound Propagation through Attenuative Elastic Media*

For a general anisotropic material and Ndifferent relaxation processes, the stress-strain constitutive law corresponding to a Christensen's attenuative medium is assumed to be [17]:

$$\sigma_{ij} + \sum_{k=1}^{N} a_{k,ijmn} \frac{d^k \sigma_{mn}}{dt^k} = \sum_{k=0}^{\infty} b_{k,ijmn} \frac{d^k \varepsilon_{mn}}{dt^k}, \tag{3.2.1}$$

where $\varepsilon_{mn} = \frac{1}{2}(\frac{\partial w_m}{\partial x_n} + \frac{\partial w_n}{\partial x_m})$ and σ_{ij} are the corresponding element of the strain and stress tensors, respectively, while $a_{k,ijmn}$and $b_{k,ijmn}$are coefficients related to the material properties of the medium. For materials described by a monorelaxation process, the Christensen's constitutive law (1) particularizes into the Zener's equation [18]:

$$\sigma_{ij} + \tau_{\varepsilon,ijmn}\sigma_{mn} = S_{ijmn}\varepsilon_{mn} + \eta_{ijmn}\dot{\varepsilon}_{mn} = S_{ijmn}(\varepsilon_{mn} + \tau_{\sigma,mnkl}\dot{\varepsilon}_{kl}) \tag{3.2.2}$$

where $\tau_{\varepsilon,ijmn}$ and $\tau_{\sigma,mnkl}$ are the elements of the tensors of relaxation times of stresses and strains under constant strains and stresses, respectively, while S_{ijmn} and η_{ijmn} are the elements of the tensors of elastic constants and dynamic viscosity, respectively.

The wave equation for an attenuative material can be derived from the Cauchy-Newton equation: $\rho\ddot{w}_i = \frac{\partial \sigma_{ik}}{\partial x_k} \quad (i,k = 1,3)$, whereρ is the material density. For the monochromatic waves, using the complex wave function: $\bar{w}\,(x,t) = \bar{w}_0 \cdot e^{j\left(\omega t - \bar{k}x\right)}$, one obtains the following differential equation in Christensen's media:

$$\rho\ddot{\bar{w}} = \bar{S} \cdot \bar{w}", \tag{3.2.3}$$

where the complex elasticity modulus $\bar{S}\,(\omega)$ is given by expression:

$$\begin{aligned} \bar{S}(\omega) &= S\left[1 - N + \sum_{i=1}^{N} \tfrac{1+j\omega\tau_{i\sigma}}{1+j\omega\tau_{i\varepsilon}}\right] = \\ &= S\left[1 - N + \sum_{i=1}^{N} \tfrac{1+\omega^2\tau_{i\sigma}\tau_{i\varepsilon}}{1+\omega^2\tau_{i\varepsilon}^2} + j\sum_{i=1}^{N} \tfrac{\omega(\tau_{i\sigma}-\tau_{i\varepsilon})}{1+\omega^2\tau_{i\varepsilon}^2}\right] = \\ &= S'(\omega) + jS"(\omega)\ . \end{aligned} \tag{3.2.4}$$

Using Equation (3.2.1), one obtains a third order differential equation, which in the homogeneous 1-D case becomes: $\rho\,(\ddot{w} + \tau_\varepsilon w) = S\,(w" + \tau_\sigma \dot{w}")$, where the Zener's media frequency independent parameters [19]: relaxation times under constant strains τ_ε and stresses τ_σ, respectively and relaxed elasticity modulus $S\,(\equiv M_R)$ are replaced for

Christensen's media by the corresponding *effective parameters*, given by the following frequency functions:

$$\begin{aligned}
\tau_{\varepsilon}(\omega) &= \frac{1}{\omega}\cdot\frac{Im\prod\limits_{i=1}^{N}(1+j\omega\tau_{i\varepsilon})}{Re\prod\limits_{i=1}^{N}(1+j\omega\tau_{i\varepsilon})},\\
\tau_{\sigma}(\omega) &= \frac{1}{\omega}\cdot\frac{Im\left\{(1-N)\prod\limits_{i=1}^{N}(1+j\omega\tau_{i\varepsilon})+\sum\limits_{i=1}^{N}\left[(1+j\omega\tau_{i\sigma})\prod\limits_{k\ (\neq i)}^{1,N}(1+j\omega\tau_{k\varepsilon})\right]\right\}}{Re\left\{(1-N)\prod\limits_{i=1}^{N}(1+j\omega\tau_{i\varepsilon})+\sum\limits_{i=1}^{N}\left[(1+j\omega\tau_{i\sigma})\prod\limits_{k\ (\neq i)}^{1,N}(1+j\omega\tau_{k\varepsilon})\right]\right\}},\\
S(\omega) &= M_R\frac{Re\left\{(1-N)\prod\limits_{i=1}^{N}(1+j\omega\tau_{i\varepsilon})+\sum\limits_{i=1}^{N}\left[(1+j\omega\tau_{i\sigma})\prod\limits_{k\ (\neq i)}^{1,N}(1+j\omega\tau_{k\varepsilon})\right]\right\}}{Re\prod\limits_{i=1}^{N}(1+j\omega\tau_{i\varepsilon})}.
\end{aligned}\qquad (3.2.4)$$

The use of *the effective Zener parameters* given by the expressions (3.2.4) simplifies considerably the description of the harmonic waves propagation through real (Christensen's) media, but the corresponding Finite Differences (FD) simulations remain unstable because the complex wave equation (3.2.3) has: (i) 4 distinct mathematical solutions: $\bar{w}=Ae^{\pm j\omega t}\cdot\exp\left[\pm j\left(k-j\alpha\right)x\right]$, a unique solution corresponding to the physical (attenuated progressive) wave, and the other 3 parasitic solutions cannot be avoided by the numerical simulations, (ii) complex solutions, whose real and pure imaginary parts mix during the FD iterations, leading to a quick increase of the computing errors and to the instability of the corresponding FD schemes. Taking into account that for a given frequency, only 2 parameters (e.g. the real S' and pure imaginary S'' parts of the complex stiffness) are independent, it is possible to simplify more the description of the harmonic waves propagation through real (Christensen's) attenuative media.

So, taking into account the definition of the tangent of the angle of mechanical losses: $\tan\delta(\omega)=\frac{Im\left[\bar{S}(\omega)\right]}{Re\left[\bar{S}(\omega)\right]}$,the complex wave equation (3.2.3) becomes:

$$\frac{\partial^2\bar{w}}{\partial x^2}=\frac{\rho}{\bar{S}}\cdot\frac{\partial^2\bar{w}}{\partial t'^2}=\frac{\rho\cdot\cos\delta}{S}\cdot e^{-i\delta}\cdot\frac{\partial^2\bar{w}}{\partial t'^2}=\frac{\rho\cdot\cos^2\delta}{S}\left(1-j\cdot\tan\delta\right)\frac{\partial^2\bar{w}}{\partial t'^2}\quad .$$

Denoting: $R=\rho\omega\cdot\tan\delta$ (*the viscous friction coefficient*), and taking into account that for harmonic waves: $\ddot{\bar{w}}=j\omega\,\dot{\bar{w}}$, it results that the above complex wave equation can be written as:

$$S_o\bar{w}"=\frac{\left|\bar{S}\right|}{\cos\delta}\cdot\bar{w}"=\rho\left(1-j\cdot\tan\delta\right)\frac{\partial^2\bar{w}}{\partial t'^2}=\rho\frac{\partial^2\bar{w}}{\partial t'^2}+R\frac{\partial\bar{w}}{\partial t'}$$

(because for Maxwell's media: $S_o=M_U$ (*the unrelaxed elasticity modulus*), for general Christensen's media S_o can be named *the Rayleigh-Stokes (pseudo unrelaxed) elasticity modulus*).

The differential equation (30) can be decomposed in its real and pure imaginary parts, obtaining the real wave equation:

$$\rho\frac{\partial^2 w}{\partial t'^2}+R\frac{\partial w}{\partial t'}=S_o w". \tag{3.2.5}$$

Taking into account that equation (3.2.5) has: (i) a unique parasitic solution (corresponding to its symmetry relative to the space inversion: $x\rightarrow$ -x), (ii) does not produce any mixture of the real and pure imaginary components of the complex wave function, it represents the best starting point for FD simulation schemes, the stability and accuracy of the corresponding FD schemes being – for these reasons – the best possible [20].

b) *Effective Parameters Specific to the Low Frequency Dynamic Magnetization of the Ferro- and Ferrimagnetic Materials*

During the last years, due to the technical interest presented by the use of the ferro- and ferrimagnetic materials in circuits of alternating current, one finds the increase of the interest for the determination of the physical parameters of the dynamic magnetization of these materials.

In the field of low frequencies, there are mainly used: *the method of the RLC bridge* ([21]) for the determination of the initial permeability and of the parameters of the dynamic magnetization in fields of low intensity and *the methods of the "sinusoidal forced" magnetic field strength* (of the electrical current in the first winding) [22] and *of the "sinusoidal forced" magnetic induction* (voltage on the second winding) [23], [21d], resp. for the evaluation of the parameters of the dynamic hysteresis cycle.

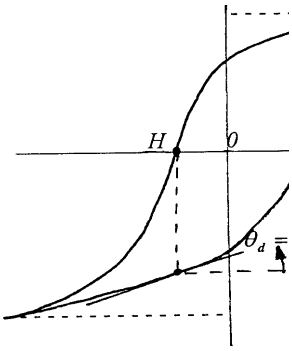
Taking into account that the magnetic field strength inside the (toroidal, usually) sample depends on position, the physical parameters of the dynamic magnetization of the sample (permeability, tangent of the angle of magnetic losses, magnetic induction, etc) depend also on the position, as well as on time during the period of the electrical current through the first winding. Consequently, *the values given for these parameters by the relations indicated by the specified works* represent averages of the distribution values, obtained in different conditions (often very difficult to be described analytically), therefore *they do not correspond to the same magnetization state of the same volume element of the considered sample*, as it is assumed usually.

E.g., the values of the maximum magnetic induction determined by the method of the sinusoidal electrical current (B_{oi}) and of the sinusoidal voltage (B_{ou}), respectively, are given by the expressions:

$$\begin{aligned} B_{ou} &= \frac{e}{2\pi f N_s h(r_e-r_i)}=\frac{\Phi_o}{N_s h(r_e-r_i)}=B_{oi}=\frac{1}{r_e-r_i}\int_{r_i}^{r_e}B_o(r)= \\ &= \frac{N_f}{4\pi(r_e-r_i)}\int_{r_i}^{r_e}\left[\int_{-I_o}^{I_o}\mu_{dr}\left(\frac{N_f I}{2\pi r},\frac{N_f I_o}{2\pi r}\right)\cdot dI\right]\frac{dr}{r}\ , \end{aligned}$$

where r_e, r_i, h are the outer and the inner radii, resp. and the height of the toroidal (with rectangular section) magnetic sample. N_f and N_s are the numbers of turns

of the first and of the second winding, resp., I_o is the amplitude of the alternating current (of frequency f) in the first (primary) winding and $\mu_{dr}(H, H_o)$is the function describing the dependence of the differential permeability on the remagnetization branch of the dynamic hysteresis cycle (fig. 3.2) on the amplitude H_o and



the momentary value $H(t)$ of the magnetic field strength.
In the particular case of the Rayleigh's domain ($H \sim H_c/10 << H_c$):

$$B = \mu_i H + \quad R.H^2, \tag{3.2.6}$$

the above expression gives, for the (frequent) case $r_e \approx 2r_i$:

$$B_{ou} = B_{oi} \cong \frac{3}{2} \ln 2 \cdot \mu_i H_{om} + \frac{9R}{8} \cdot H_{om}^2 \ ,$$

with:

$$H_{om} = \frac{N I_o}{\pi \left(r_e + r_i \right)} \ . \tag{3.2.7}$$

The relation (3.2.7) shows that the value of the amplitude of the magnetic induction ($B_{ou} = B_{oi}$) associated – by the present theory of the dynamic magnetic measurements – to the "average" amplitude H_{om} of the magnetic field strength in the toroidal sample is, even for the Rayleigh's domain, larger with *4.1 ... 12.5%* than the real (physical) value corresponding to this magnetic field strength:

$$B_{om} = \mu_i H_{om} + R \cdot H_{om}^2 \quad .$$

The errors become even larger in the field of the strong dependence of the magnetic permeability on the magnetic field strength (for $H \sim H_c$), being in this case of the magnitude order of 10% or even larger.

For this reason, *a reconsideration of the procedure used for the evaluation of the parameters of the dynamic magnetization of the ferri- and ferromagnetic materials is necessary now.* It results also that for a more rigorous evaluation of the (effective)

parameters of the dynamic magnetization of the considered materials, a previous study of the dependence $\mu_{dr}(H, H_o)$is necessary. In fact, starting from this dependence, it is possible to find all other important features of the dynamic magnetization: (i) *the maximum induction* (flux density):

$$B_0(H_0) = \frac{1}{2} \int_{-H_0}^{H_0} \mu_{dr}(H, H_0) dH, \tag{3.2.8}$$

(ii) *the differential permeability on the plot of first magnetization* (μ_{diff}),*the total permeability* (μ_{tot}) *and the initial one* (μ_i):

$$\mu_{diff} = \frac{dB_0}{dH_0} \quad , \qquad \mu_{tot} = \frac{B_0}{H_0} \quad , \qquad \mu_i = \lim_{H_0 \to 0} \mu_{diff} = \lim_{H_0 \to 0} \mu_{tot} \ , \tag{3.2.9}$$

(iii) *the equations of the branches of de- and remagnetization of the dynamic hysteresis cycle:*

$$B_d(H, H_0) = B_0 - \int_{H}^{H_0} \mu_{dr}(-, H_0) dH, \qquad B_r(H, H_0) = B_0 - \int_{H}^{H_0} \mu_{dr}(H, H_0) dH, \tag{3.2.10}$$

(iv) *the values of the remanent induction (flux density) and of the coercive field:*

$$B_{rem}(H_0) = \int_{0}^{H_0} \mu_{dr}(H, H_0) dH \ - B_0, \qquad \int_{H_c}^{H_0} \mu_{dr}(H, H_0) dH = B_0, \tag{3.2.11}$$

with:

$$B_r = \lim_{H_0 \to \infty} B_{rem}(H_0), \qquad H_c = \lim_{H_0 \to \infty} H_c(H_0), \tag{3.2.12}$$

v) *the saturation magnetization:*

$$M_{sat} = \lim_{H_0 \to \infty} \left[\frac{B_0 \left(H_0 \right)}{\mu_0} - H_0 \right], \quad etc \tag{3.2.13}$$

The macroscopic (electrical engineering) effective parameters can be expressed also by means of the remagnetization differential permeability. Truly, in the usual case of the Owen and Maxwell's bridges, the inductance of the magnetic sample is determined by the voltage equilibration (compensation) on the inductive reactance:

$$L \frac{dI}{dt} = (< L > + \delta L) \frac{dI}{dt} \quad ,$$

where $< L >$is the time average of the inductance and δL is the inductance fluctuation around its mean value. Taking into account that the time average of the product

$\delta L.dI/dt$ is null, it results that the measured (effective) value of the inductance is:

$$\begin{aligned} L_m(I_0) &=< L(I_0) >= \tfrac{2}{T}\int\limits_0^{T/2} \tfrac{d\Phi}{dI}\cdot dt = \tfrac{2N}{T}\int\limits_0^{T/2}\left[\int\limits_{r_i}^{r_e}\tfrac{dB}{dH}\cdot\tfrac{dH}{dI}\cdot dr\right]dt = \\ &= \tfrac{N^2h}{T}\cdot\int\limits_0^{T/2}\left[\int\limits_{r_i}^{r_e}\mu_{dr}\left(\tfrac{NI}{2\pi r},\tfrac{NI_0}{2\pi r}\right)\tfrac{dr}{r}\right]dt\ . \end{aligned} \tag{3.2.14}$$

Similarly, the resistance of the hysteresis losses can be expressed by means of the dissipated power P_h during a hysteresis cycle under the action of a magnetic field generated by an electrical current (in the primary winding) of frequency f and amplitude I_0:

$$R_h = \frac{2P_h}{I_0^2} = \frac{4\pi hf}{I_0^2}\int\limits_{r_i}^{r_e} r\left\{\int\limits_{-H_0}^{H_0}\left[B_d(H,H_0)-B_r(H,H_0)\right]dH\right\}dr, \tag{3.2.15}$$

and the maximum value u_C of the voltage on the integration condenser (the method of the sinusoidal forced current) and the effective value e_{eff} of the induced voltage in the secondary winding (the method of the sinusoidal forced voltage) are obtained by means of relations:

$$u_C = \frac{hAN_s}{\tau}\int\limits_{r_i}^{r_e} B_0(r)dr, \qquad e_{eff} = \sqrt{2}\pi f N_s\int\limits_{r_i}^{r_e} B_0(r)dr, \tag{3.2.16}$$

where τ is *the time constant of the integrator* and $A$is *the amplification factor.*

c) *Effective Parameters specific to the Intramolecular Structures and Interactions*

It is well-known that different physical methods used in Molecular Physics involve averages of different types of the molecules velocities: (i) the coefficient of the thermal conduction can be expressed by means of the cubic mean velocity of molecules, (ii) the internal energy of gases is expressed in terms of the mean square velocity, (iii) the most probable distance (from the "geometrical shadow") of the Ag atoms deposed on the external cylindrical surface of a Stern installation can be expressed by means of the most probable inverse velocity of molecules: $1/¡1/v¿_{mp}$ and so on. Because the characteristic molecular velocities present a certain order:

$$\sqrt[3]{< v^3 >} > \sqrt{< v^2 >} > \tilde{v} > v_{mp} > \frac{1}{< 1/v >} > ..., \tag{3.2.17}$$

it results that the effective (characteristic) molecular velocities have distinct values and must be studied separately.

These findings are valid also for the effective parameters of the (intra)molecular structures and interactions. So, taking into account that the distance between the

successive spectral lines of the pure rotation (microwave) spectrum of the diatomic molecules is:

$$\Delta\nu = \frac{h}{8\pi^2\mu r^2} \tag{3.2.18}$$

(where μ=$m_1m_2/(m_1+m_2)$ is *the effective mass of the diatomic molecule* and r is the distance between its atomic nuclei), it results that *the effective distance between the atomic nuclei* of a diatomic molecule, determined starting from the microwave spectrum data, is an inverse square mean average of the distances between these atomic nuclei:

$$r_{MS} = \frac{1}{\sqrt{<\frac{1}{r^2}>}}. \tag{3.2.19}$$

For this reason, the numerical results (referring to the distances between the atomic nuclei) obtained by means of the pure rotation (microwave) spectra and of the electron diffraction, will be systematically different, because the last ones correspond to the average distance $r_{ED} =< r >$.

Taking into account that besides the classical methods based on: (i) the microwave spectra and: (ii) the electron diffraction, there are several additional methods which allow also the evaluation of some effective parameters of the (intra)molecular structure and interactions (mainly, the methods using: (iii) the fine structure of the nuclear resonance spectrum (NMR), (iv) the molecular orbitals (MO), (v) the vibration spectra of the first 3 orders, (vi) the rotation structure of the vibration bands, (vii) the collections of deformation constants (by means of the so-called conformational analysis) etc, as well as that the averages of the molecular parameters (geometrical or specific to interactions) over the intramolecular "motions" are specific to each experimental method, the main features of the determined effective parameters depend strongly on the used experimental method. That is why a synthesis of the main features of the effective parameters characteristic to the (intra)molecular "geometrical" structure and interactions is presented in the following Tables 3.1 and 3.2.

Content of the future monograph "Elements of Numerical Physics"

The above 14 pages present in detail the main elements of the first 2 chapters, as well as of the first 2 paragraphs of the projected monograph. Taking into account the finite volume of this abstract, we must present in following only the basic details concerning the content of the projected monograph.

Besides its first 2 paragraphs above presented, **Chapter 3 "Specific Problems of the Numerical Physics"** will involve also the following paragraphs:

§3.3. Some statistical tests specific to Physics (in frame of this paragraph, will be presented briefly some of the main statistical tests of: a) large data volume (the tests: (i) χ^2 (Pearson), (ii) Kolmogorov, (iii) Smirnov-Grubbs etc), b) small data volume (the tests of: (i) Massey, (ii) Irwin, (iii) Sarkady etc), as well as some statistical tests intended to the elimination of the plunder experimental errors (the tests of: (i) Chouvenet, (ii) Charlier etc))

§3.4. Finding out of the similitude criteria and domains (some examples specific to fluid flows, heat exchange, as well as to some classical Physics fields)

§3.5. Procedures for the obtainment and study of semiempirical relations

§3.6. Procedures used for the obtainment of the confidence intervals and for the study of the compatibility of some theoretical (or semiempirical) relations relative to the existing experimental data

§3.7. Possibilities of evaluation of the apparent and real information amounts, respectively, and of their use in some Physics problems (the delimitation of the real physical information and of the misinformation, as well as of the possibilities to measure the real information, will be analyzed)

§3.8. Some Numerical Methods specific to Physics (the main analyzed Numerical Methods will be: a) the Finite Differences method [24] and its form (the Local Interaction Simulation Approach (LISA) method [25]) specific to Physics and to the use of parallel computers), b) the search methods used to solve the so-called "*inverse problems*", mainly: (i) the deterministic search methods (the gradient (Jacobi's) method etc), (ii) the random methods (the Monte Carlo method, the random walk method etc), (iii) the intermediate methods (the method of genetic algorithms and others) etc.)

§3.9. Numerical Phenomena Specific to some Numerical Methods (there will be analyzed mainly the numerical phenomena specific to: a) the FD method (mainly the phenomena of: (i) instability, (ii) divergence, of pseudoconvergence, inclusively [26], (iii) dispersion, involving the main aspects concerning the possible distortions, as well as the causes which lead to such numerical phenomena in certain particular Physics problems [27], b) the gradient method (mainly the phenomena of: (i) oscillations, (ii) instability, (iii) misinformation due to the incorrect choice of the zero-order approximations of the uniqueness parameters, etc)

Chapter 4 "Specific Technical Applications" will have the following content:

§4.1. Uniparametric Technological Series of Industrial Materials (besides the presentation of such series, the derivation of some "limit laws" (valid for magnetic materials, dielectric materials etc), as well as their applications will be also discussed)

§4.2. Design of the Laboratory Experiments and of the Similitude Laboratory Models of Some Industrial Installations (this paragraph will refer mainly to the design principles of the laboratory experiments and to the construction principles of the similitude laboratory models, and it will present also some examples (e.g. for the experimentation of cryogenic cables))

§4.3. Optimization of the design of some technical or/and scientific devices and installations (some elements concerning the optimization principles and examples concerning some devices of magnetic measurements)

§4.4. Numerical Simulations of some Physical Processes in Inaccessible Conditions (it is underlined that these numerical simulations are useful even in

the case of some accessible, but expensive conditions, due to the considerably lower (practically negligible) costs of the numerical simulations)

§4.5. Elaboration of some Physical Models intended to the Applications of the Systems Theory (taking into account that the well-elaborated Systems Theory needs always detailed physical models of the studied systems in order to be applied)

Finally, the **Chapter 5 "Specific Didactic Applications"** will have the content:

§5.1. Classification of the main Physics domains by means of the Similitude Criteria (there will be analyzed: a) the delimitations of the: (i) nonrelativistic, relativistic, and extreme relativistic Physics, (ii) classical and Quantum Physics, (iii) classical (Newtonian) and Einstein's gravitation theories, b) the similitude criteria in other Physics fields: (i) Elasticity Theory and Sound Waves, (ii) Thermodynamics of Irreversible Phenomena, (iii) Electromagnetism, (iv) Electromagnetic Waves, (v) Quantum Physics, (vi) Condensed Matter Physics)

§5.2. Classification of the physical parameters by means of the method of Physics symmetries (the definitions of the: a) scalar (with particular cases of the: (i) proper, (ii) improper types), b) vector (particular cases of the: (i) polar, (ii) axial types), c) tensor (particular cases of: (i) proper, (ii) pseudo types) parameters will be presented and some examples concerning the consequences and the applications of these notions will be discussed)

§5.3. Elements about the main physical analogies (mainly the analogies corresponding to: a) the analytical formalism of Physics, b) the Physics thermal and statistical formalisms, c) the wave formalism)

§5.4. Logical Schemes intended to the Physics study and learning (we want to present both: a) some general logical schemes intended to: (i) the (General) Physics study, (ii) Data Processing, etc and: b) logical schemes ("maps") intended to the study of some particular Physics domains, as: (i) the Relativity Theory, (ii) the Quantum Physics, etc)

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Table 1. Comparison between the present physical methods used to determine the complete (and nonperturbed) molecular structure

INPUT DATA	**THE STRUCTURE**	**THE COMPARISON CRITERION**				
		Are there used semi-empirical relations for data processing ?	Reproducibility of the results from different sets of experimental data ($\Delta M/M$)*	Magnitude order of the relative difference in respect to the equilibrium molecular configuration $((r - r_{equil.})/r)$*	Possibilities of refinement of the effective structure towards the equilibrium configuration; are there necessary some semiempirical relations ?	Is the space of the effective structure linear ?
Microwave Spectra	of substitution (r_s)	NO	$< 10^{-3}$	$< 10^{-2}$	YES; -	YES
	classical (r_o)	NO	$< 5 \times 10^{-2}$	$< 5 \times 10^{-2}$	YES; -	YES
	average (r_z)	NO	$< 2 \times 10^{-3}$	$< 2 \times 10^{-2}$	YES; -	YES
Electronic Diffraction Spectra	of radial distribution (r_g (1))	YES	$< 2 \times 10^{-3}$	$< 2 \times 10^{-2}$	YES; -	YES
	$r_g(0)$	YES	$< 3 \times 10^{-3}$	$< 5 \times 10^{-2}$	YES; YES	NO
Fine structure of NMR Spectrum	of nuclear magnetic coupling (r_J)	YES	$< 5 \times 10^{-2}$	$< 5 \times 10^{-2}$	NO	NO
Molecular Orbitals	r_{MO}	YES	$< 2 \times 10^{-2}$	$< 3 \times 10^{-2}$	Difficult; nonsure	NO
Collection of deformation constants	of conformational analysis (r_{CA})	YES	$< 5 \times 10^{-2}$	$< 5 \times 10^{-2}$	NO	YES

* Estimated values starting from the data of the specialty literature, as well as from the original analytical relations established in Section I.2.

Table 2. Comparison of the present methods of determination of the effective intramolecular force fields

INPUT DATA	FORCE FIELD	THE COMPARISON CRITERION						
		Are there used semi-empirical relations in data processing ?	Reproducibility of the results $(\Delta M/M)$*	Relative differences of the calculated relative to the experimental frequencies $((\nu_{calc} - \nu_{exp})/\nu_{exp})$*	Are there possibilities of obtainment of the structural parameters and of the complete force field ?	Is there a multiplicity of solutions ?	Number of independent parameters of the force field	Special disadvantages of the method
Vibration Spectra of the orders 1, 2 and 3	UAQFF	NO	$< 10^{-2}$	$< 10^{-2}$	NO	YES	$N_v(N_v+1)/2$	
	EAQFF	NO	$< 3.10^{-3}$	$< 3.10^{-3}$	YES; YES	YES	$N_v\ (N_v+1)/2$	
	Complete (up to the quartic terms, inclusively)	NO	Quadratic component $< 2.10^{-3}$ The others $< 10^{-2}$	$< 10^{-3}$	YES; YES	YES	$\sim N_v^4$	
	Urey-Bradley with elimination of anharmonicities	NO	$< 5.10^{-3}$	$< 5.10^{-3}$	NO; YES	YES	$\sim 2N_v$	
	Method of generalized isotopic substitutions	NO	$< 3.10^{-3}$	$< 3.10^{-3}$	YES; YES	NO	$N_v\ (N_v+1)/2$	Many input data (difficult to be collected)
Rotation structure of Vibration bands	Method of Coriolis coefficients	NO	$< 10^{-2}$	$< 5.10^{-3}$	YES; NO	YES	$N_v\ (N_v+1)/2$	Very difficult calculations
Fine (sharp) Structure of NMR Spectra	Method of Coupling Constants	YES	$< 2.10^{-2}$	$< 2.10^{-2}$	NO; NO	NO	$\sim\ N_v$	
Molecular Orbitals	k_{MO}	YES	$< 10^{-2}$	$< 10^{-2}$	Difficultly	NO	$N_v\ (N_v+1)/2$	

* Estimated values by means of the specialty literature data.