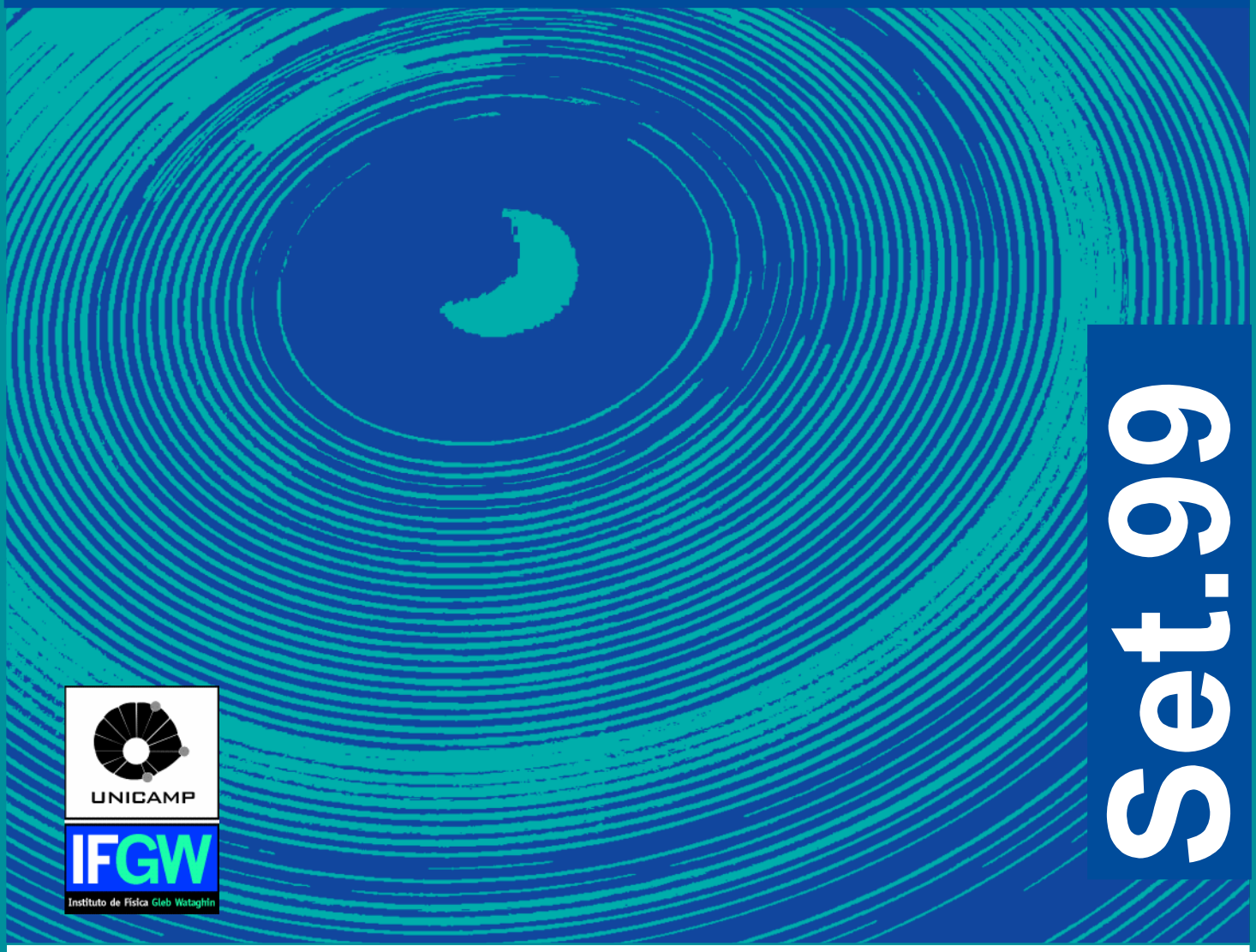
Abstracta

Ano III - N. 08



Trabalhos Aceitos para Publicação

A045-99 à A051-99

Trabalhos Aceitos para Publicação em Conferências

C004-99

Accepted papers

[A045-99] "Landau Level Quantization and Possible Superconducting Instabilities in Highly Oriented Pyrolitic Graphite."

Y. Kopelevich, V. V. Lemanov, S. Moehlecke, J. H. S. Torres

Measurements of the basal-plane resistivity r a (T,H) performed on highly oriented pyrolic graphite, with magnetic field H ll c-axis in the temperature interval 2 K - 300 K and fields up to 8 T, provide evidence for the occurrence of booth field-induced and zero-field superconducting instabilities. Additionaly, magnetization M(T,H) measurements suggest the occurrence of Fermi surface instabilities which complete with the superconducting correlations.

Physics of the Solid State 41 (12), 13, 1999

[A046-99] "A Nonequilibrium Statistical Ensemble Formalism, MaxEnt-NESOM: Basic Concepts, Construction, Application, Open Questions and Criticism."

R. Luzzi, A. R. Vasconcelos, J. Galvão Ramos

We describe a particular approach for the construction of a nonequilibrium statistical ensemble formalism for the treatment of dissipative many-body systems. This is the so-called Nonequilibrium Statistical Operator Method, based on seminal and fundamental ideas set forward by Boltzmann and Gibbs. The existing approaches can be unified under a unique variational principle, namely, MaxEnt, which we considerer here. The main six basic steps that are the at foundations of formalism are presented and the fundamental concepts are discussed. The associated nonlinear quantum kinetic theory and the accompanyng Statistical Thermodynamics (the Informational Statistical Thermodynamics) are very briefly described. The corresponding response function theory for systems away from equilibrium allows to conected the theory with experiments, and some examples are summarized; there follows a good agreement between theory and experimental data in the cases in which the latter are presently available. We also present an overview of some conceptual questions and associeted criticisms.

Los Alamos National Laboratory Eletronic File: cond-matt - 9909160 , 11 set 1999, <http://xxx.lanl.gov=cond-mat=9909160>

[A047-99] "Structure-Activity Relationship Studies of Carcinogenic Activity of Polycyclic Aromatic Hydrocarbons Using Calculated Molecular Descriptors with Principal Component Analysis and Neural Network Methods."

R. Vendrame, R. S. Braga, Y. Takahata, D. S. Galvão

Recently a new methodology based on local density of state calculations(LDOS) using topological and semi-empirical methods was proposed to identify the carcinogenic activity of polycyclic aromatic hydrocarbons (PAHs). In this work we perform a comparative study of this methodology with principal component analysis (PCA) and neural networks (NN). The PCA and NN results show that LDOS quantum chemical descriptors are relevant descriptors to identify the carcinogenic activity of methylated and non-methylated PAHs. Also, we show that the combination of these distinct methodologies can be an efficient and powerful tool to the structure-activity studies of PAHs compounds. We have studied 81 methylated and non-methylated PAHs and our study show that with the use of these methods it is possible to correctly predict the carcinogenic activity of PAHs with accuracy higher than 80%.

Journal of Chemical Information and Computer Science 39 (6), 1094-1104, 1999

[A048-99] "Entanglement and Nonextensive Statistics."

A. Vidiella-Barranco

It is presented a generalization of the von Neumann mutual information in the context of Tsallis' nonextensive statistics. As an example, entanglement between two (two-level) quantum subsystems is discussed. Important changes occur in the generalized mutual information, which measures the degree of entanglement, depending on the entropic index q.

Physics Letters A 260 (5), 335-339, 1999

[A049-99] "Eletronic Indices from Semi-Empirical Calculations To Identify Carcinogenic Activity of Polycyclic Aromatic Hydrocarbons."

P. M. V. B. Barone, R.S. Braga, A. Camilo Jr., D. S. Galvão

Recently we have shown that it is possible to group and identify the carcinogenic activity of the polycyclic aromatic hydrocarbons (PAHs) using very simple rules derived from simple Hückel calculations. In this work we have carried out similar calculations using semiempirical methods in order to investigate whether the derived rules are method dependent. We present PM3 (Parametric Method 3) and ZINDO-CI (Zerner Intermediate Neglect of Differential Overlap - Configuration Interaction) study on the electronic structure of PAHs. Very similar rules, based on the concept of electronic local density of states over specific molecular regions, are derived from PM3 calculations showing that they are essentially method independent. The analysis of the ZINDO-CI results for the intensity of the threshold transitions (first optical transitions) and the composition of the CI contributions also show a differentiated behavior for the strong carcinogenic molecules and the inactive ones.

Journal of Molecular Structure (THEOCHEM) 505 (1-3), 55-66, 2000

[A050-99] "Optimized Electrolyte for Electrochemical Capacitance-Voltage Profiling of Carrier Concentration in In0.49Ga0.51P."

A. Da Silva Filho, N. C. Frateschi

Electrolyte characterization and optimization for the electrochemical capacitance-voltage profiling of carrier concentration in In0.49Ga0.51P is presented. The conditions for operation under minimum electrolyte interference are found based on the complex impedance analysis of an electrolyte-semiconductor junction. Carrier concentration results obtained with the optimized electrolyte are shown to both provide good etch depth control and to agree with Hall measurements. The same optimization scheme may be used for the characterization of other semiconductor material.

Journal of Electronics Materials 28 (12), 1428-1432, 1999

[A051-99] "Optical Properties of Nonequilibrium Low-dimensional Systems."

S. A. Hassan, A. R. Vasconcellos, M. V. Mesquita, R. Luzzi

The optical properties of low-dimensional carrier systems ("quantum wire"-type) driven away from equilibrium are studied. The frequency and wavevector-dependent dielectric function of a quasi-one-dimensional electron system under the action of an exciting external pumping source is derived. The optical responses of the systems are obtained in terms of its nonequilibrium thermodynamic state, the latter characterized resorting to a nonequilibrium statistical ensemble formalism.

Physical Review E 61 (1), 71-76, 2000

Accepted papers for conference presentation

C 004-99 "Considerations on Fröhlich Synchronous Large-Scale Collective Oscillations: Fröhlich-Bose-Einstein Condensate."

R. Luzzi

Normal vibrations in large biomolecules (biopolymers) have frequencies typically in the GHz/THz range and they are usually associated with oscillating electric polarization. A related and particularly interesting question, associated with complex behavior and transport of signals in biosystems, is the so-called Fröhlich effect and the propagation of Schrödinger-Davydov solitary waves. Both phenomena appear to be of relevance in Bioenergetics. Fröhlich effect consists in that, once a critical level of pumping of metabolic energy is attained, there follows the emergence of a self-organized dissipative structure resembling a nonequilibrium Bose-Einstein-like condensation in the low-lying in frequency modes of vibration. On the other hand, the Schrödinger-Davydov soliton lifetime, which is short in normal physiological conditions, becomes very large when propagation accurs in Fröhlich condensate. Further complex behavior in a Fröhlich condensate of acoustical vibrations, apparently present in ultrasonic medical imaging, and dubbed Fröhlich-Cherenkov effect is also considered.

In: Workshop on Applications and Exploitations of Microwave Space Core Technologies, Brasil-United Kingdow Joint Project, São Paulo, Brasil, Sept, 1999

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Abstracta

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