Abstracta

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Trabalhos Aceitos para Publicação

A001-97 à A002-97

Trabalhos Submetidos à Publicação

P001-97 à P004-97

Accepted papers

[A001-97] "Feynman Identity: a special case. I"

G.A.T.F. da Costa

There is an identity due to Feynman which relates graphs and closed curves on a lattice and it was used by Feynman in his combinatorial proof of Onsager's closed formula for the partition function of the two-dimensional Ising model. Long ago Sherman considered a special case of this identity and pointed out similarities with the Witt identity of Lie algebra theory. In this paper and following we revisit this special case and solve some problems related with it. In particular, the weights are computed explicitly using paths and words and a direct connection with Witt formula is found.

Journal of Mathematical Physics 38 (2), 1014, Fev 1997

[A002-97] "The Role of Hydrogen in Nitrogen-Containing Diamond-Like Films Studied by Photoelectron Spectroscopy."

S. Souto e F. Alvarez

The influence of H on the local structure of N-containing amorphous diamond-like films (a-CN$_x$:H) is reported. The samples were prepared by rf-sputtering of graphite in a N_2, Ar and H_2 atmosphere. The chemical bonding of C and N atoms was inferred by analyzing the C ls and N ls electronic core-level by X-ray photoelectron spcetroscopy. Hydrogen free films present Nls peaks with a "doublet", located at 398.2 eV - 400.5 eV. When H is introduced in the preparation chamber, the doublet evolves to a single wider band located at 399.1 eV. This new band becomes dominant when increasing H_2 partial pressure, completely hiding the original structure. High H_2 partial pressure interrupts the growing network formed by N and C due to the attachment of H to N and/or C. Furthermore, the experimental results suggest that the possibility of formation of the C_3N_4 phase-like is inhibited by the presence of hydrogen.

Applied Physics Letters 70 (12), 1539, Jan 1997

Submitted papers

[P001-97] "Flux Operators of Dynamical Quantities in a Nonequilibrium Statistical Ensemble Formalism."

J. R. Madureira. A. R. Vasconcellos e R. Luzzi

It is shown how the closure condition, which defines the space of nonequilibrium macroscopic states in the so-called Informational Irreversible Thermodynamics, introduces a series of fluxes of a reference set of densities. These fluxes are the average values over a Gibbs-like nonequilibrium ensemble of Hermitian operators defined at the microscopic-mechanical level. Their connection with the associated Lagrange multipliers, that the method introduces, is established. These Langrange multipliers are interpreted as drift velocities (of ever increasing tensorial order) divided by a nonequilibrium temperature-field-like variable. The equations of evolution for these fluxes (or equivalently for their conjugated Lagrange multipliers) are described. An illustrative example is given, and connection with experiment considered.

Brazilian Journal of Physics 28 (2), 122-131, Jun 1998

[P002-97] "Stratum Corneum Protein Mobility as Evaluated by a Spin Label Maleimide Derivative."

A. Alonso e M. Tabak

The molecular dynamics in the sulphydryl regions of stratum corneum (SC) proteins has been studied through electron paramagnetic resonance (EPR) spectroscopy of a maleimide spin label. We have interpreted the coexistence of two spectral components in the EPR spectra as due to the existence of two nitroxide conditions. A strongly immobilized component arises when the nitroxide is hydrogen bonded to the protein and the weakly immobilized component is due to the nitroxide dissolved in the aqueous environment. The calculated energetic gain for the nitroxide to form hydrogen bond with SC proteins was 3.8 Kcal/mol in the temperature range of 2-34 C and 1.9 Kcal/mol in the range of 34-70 C. Temperature profiles of other EPR parameters such as the linewidths of immobile and mobile components and the outer hyperfine splitting also showed changes in the temperature interval of 30-45 C, suggesting alterations in the vibration modes of SC proteins which are sensitive to higher motional freedom above 30-45 C. These results are correlated with data of lipid phase transitons and alkyl chain mobility previously observed by EPR, and support the contention that besides lipids, the SC proteins are also involved in the barrier function of SC, especially through protein-lipid interactions in the corneocyte membrane.

Biochimica et Biophysica Acta 1478 (1), 89-101, 2000

[P003-97] "The Informational-Entropy Operator in a Nonequilibrium Ensemble Formalism I: general properties."

S. A. Hassan, A. R. Vasconcellos e R. Luzzi

The Nonequilibrium Statistical Operator Method, arising out of the fundamental ideas set forward by Bogoliubov, Kirkwood, Green, Zwanzig, Mori, Zubarev and Peletminskii, among others, provides a quite promising formalism for the sought-after statistical ensemble method for nonequilibrium systems. A quantity, namely the so- called informational-statistical entropy operator, plays a fundamental role in such formalism. In the present work we report a study of this quantity, centering the attention on the determination of its eigenvalue spectrum. The latter is related to the informational entropy and its production, which are state functions in the accompanying statistical irreversible thermodynamics. Comments on the presence of a Bohr-Rosenfeld-Prigogine-like complementarity principle are presented. The particular case of a system describable in terms of single-particle states is considered, for in the follow-up article to discuss its hydrodynamic properties in terms of the results here presented.

Journal of Statistical Physics, Dez 1996

[P004-97] "The Informational-Entropy Operator in a Nonequilibrium Ensemble Formalism II: an application in hydrodynamics."
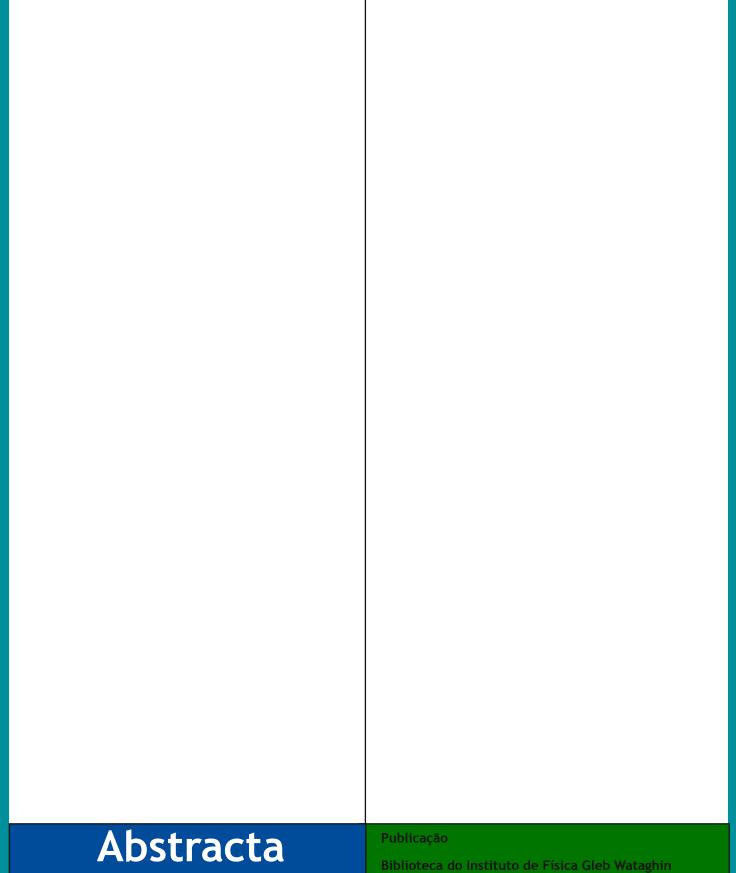
S. A. Hassan, A. R. Vasconcellos e R. Luzzi

The informational entropy operator, which has a fundamental role in the construction of a statistical irrevesible thermodynamics, had its basic properties described in the preceding article. On the basis of those results we show in the present one, as an illustrative example, how to derive a nonclassical thermo-hydrodynamics of large scope. Introducing some asymptotic limiting conditions we present some results, showing how to recover those of classical and extended phenomenological thermodynamics.

Journal of Statistical Physics, Dez 1996

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Nota: Arquivo gerado em out/2011 tendo como base as informações da edição do Abstracta distribuída na época. O arquivo original não foi preservado.

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