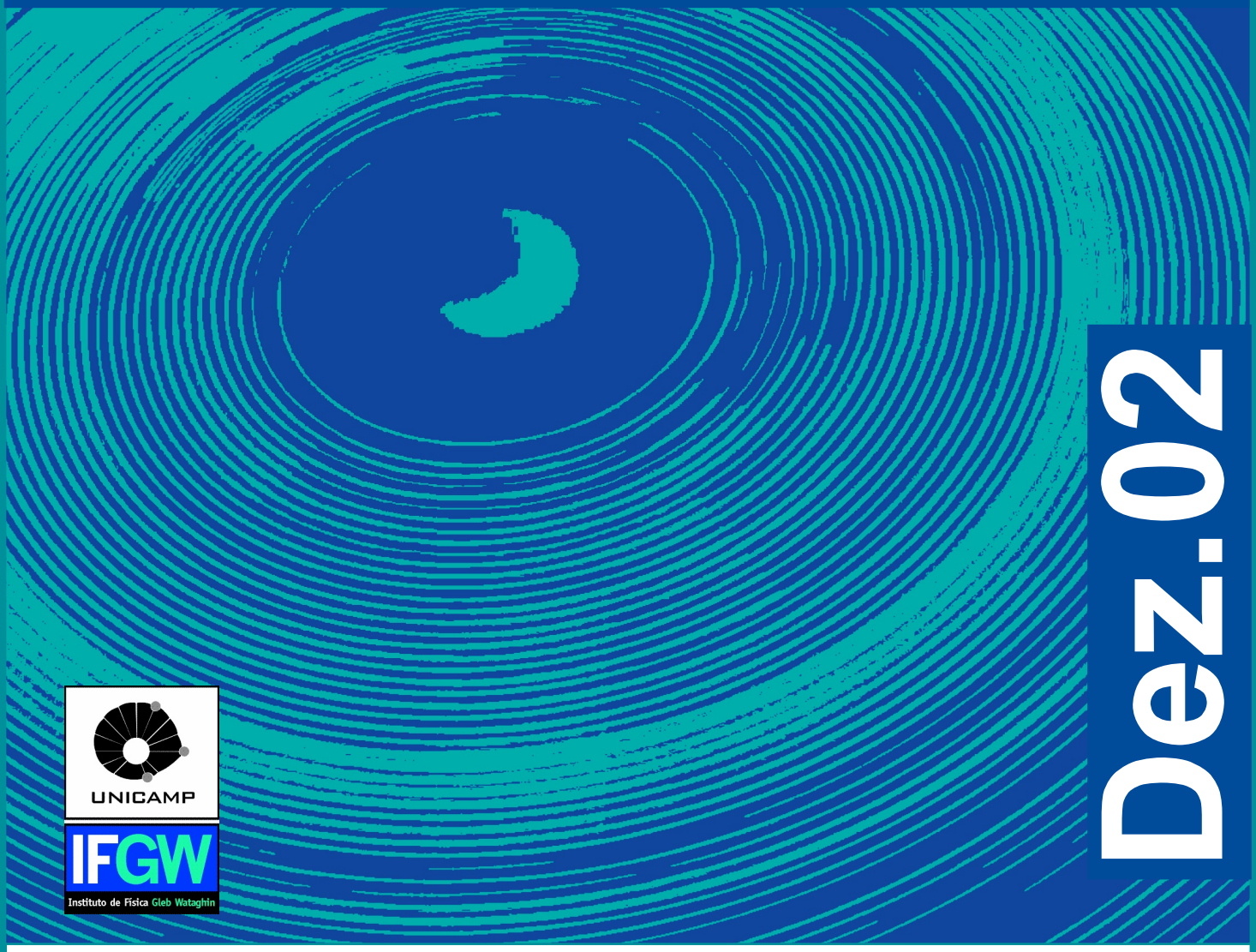
# Abstracta

Ano VI - N. 06



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## Trabalhos Publicados

P115-02 à P141-02

# TRABALHOS PUBLICADOS

**P115-02"A new approach to Auger and quasi-resonant processes in ion- surface collisions".**

**Pepino, R. T. and Kleiman, G. G.**

We present a theoretical model of charge exchange between an ion and a solid surface which includes resonant transfer and Auger-coupling processes. The Auger processes are treated through an equation of motion approach which results in an Auger self-energy identical to that obtained through the second-order Keldysh-Green functions formalism. The model which we report involves a Lorentzian-shaped level width for the resonant processes and a wide band form for the Auger processes. It permits an exact solution of the problem in terms of well-known functions. The roles played by the characteristic parameters of the problem, which are related to the atom velocity, energy level positions, interaction potential and band structure are illustrated in some simple cases. (C) 2002 Elsevier Science Ltd. All rights reserved

**Solid State Communications 124[9], 317-321. 2002.**

**P116-02"A semiempirical study on the electronic structure of 10- deacetylbaccatin-III".**

**Braga, S. F. and Galvao, D. S.**

We performed a conformational and electronic analysis for 10-deacetylbaccatin-III (DBAC) using well-known semiempirical methods (parametric method 3 (PM3) and Zerner's intermediate neglect of differential overlap (ZINDO)) coupled to the concepts of total and local density of states (LDOS). Our results indicate that regions presented by paclitaxel (Taxol(R)) as important for the biological activity can be traced out by the electronic features present in DBAC. These molecules differ only by a phenylisoserine side chain. Compared to paclitaxel, DBAC has a simpler structure in terms of molecular size and number of degrees of freedom (d.f.). This makes DBAC a good candidate for a preliminary investigation of the taxoid family. Our results question the importance of the oxetane group, which seems to be consistent with recent experimental data. (C) 2002 Elsevier Science Inc. All rights reserved

**Journal of Molecular Graphics & Modelling 21[1], 57-70. 2002.**

**P117-02"A C magnetic transport on heterogeneous ferromagnetic wires and tubes".**

**Sinnecker, J. P., Pirota, K. R., Knobel, M., and Kraus, L.**

The AC current density radial distribution is calculated on heterogeneous composite materials with cylindrical geometry. The composites have an inner core and thin outer shell that can be either from the same material (homogenous material like simple wires) or from different materials with different physical properties. The case in which a non-magnetic inner core is surrounded by a magnetic layer, like electrodeposited wires, is mainly studied. The effect of frequency and applied magnetic field is simulated. The current density distribution as a function of frequency and applied field, as well as the total current over the inner core and outer shells are calculated. The results agree substantially well with the experimentally observed data for simple electrodeposited wires. (C) 2002 Elsevier Science B.V. All rights reserved

**Journal of Magnetism and Magnetic Materials 249[1-2], 16-21. 2002.**

**P118-02"Chemical environment of copper aggregates embedded in polypyrrole films:The nature of the copper-polypyrrole interaction".**

**Watanabe, N., Morais, J., and Alves, M. C. M.**

We report on the structural and electronic properties of copper aggregates embedded in composite polypyrrole films studied by X-ray absorption techniques (XAS). Measurements at the Cu K edge during in situ reduction suggest that the reaction starts with the formation of the complex [-[(C4H2N)(3)CH3(CH2)(11)OSO3-](y)Cu2+](n) (y = 4), in which the copper is bonded to oxygen atoms. The reduction of this complex leads to the synthesis of Cu metal aggregates in the film. Measurements at, the N K edge evidence that the incorporation of the metal in the polymer network does not disturb the electronic structure nor the environment of the nitrogen from the pyrrole unit. Measurements at the 0 K edge indicate that the metal/polymer interaction happens via hybridization of O 2p and Cu 3d orbitals, resulting in an enlace that has a quasi- covalent character. Scanning electron microscopy measurements show that dendritic-like copper aggregates are formed on the film surface.

**Journal of Physical Chemistry B 106[43], 11102-11107. 2002.**

**P119-02"Comment on "Ion-assisted pulsed laser deposition of aluminum nitride thin films" [J. Appl. Phys. 87, 1540 (2000)]".**

**Zanatta, A. R., Ribeiro, C. T. M., and Alvarez, F.**

In a recent article [J. Appl. Phys. 87, 1540 (2000)] Lu have reported on the achievement of good quality crystalline aluminum nitride (AlN) films deposited on Si<100> substrates. The films were prepared in the 200-800 degreesC temperature range by the nitrogen-ion-assisted laser ablation of one AlN target. According to their experimental results, the infrared absorption bands due to Al-N bonds display a frequency shift of approx. 80 cm(-1) as a consequence of the residual stress present in the AlN films. Interestingly, and despite such a high stress, the phonon vibration modes do not exhibit any appreciable shift. Actually, most of the phonon frequencies reported by Lu perfectly match those observed in crystalline silicon. The analyses of Lu probably contain inaccuracies regarding the true crystalline quality of their AlN films and is the subject of this comment. (C) 2002 American Institute of Physics

**Journal of Applied Physics 92[10], 6349-6350. 2002.**

**P120-02"Coulomb gas approach to the anisotropic one-dimensional Kondo lattice model at arbitrary filling".**

**Novais E, Miranda E, Neto AHC, Cabrera GG**

We establish a mapping of a general spin-fermion system in one dimension into a classical generalized Coulomb gas. This mapping allows a renormalization-group treatment of the anisotropic Kondo chain both at and away from half-filling. We find that the phase diagram contains regions of paramagnetism, partial, and full ferromagnetic order. We also use the method to analyze the phases of the Ising-Kondo chain.

**PHYSICAL REVIEW B 66 (17): art. no. 174409 NOV 1 2002**

**P121-02"Designing conducting polymers using genetic algorithms".**

**Giro, R., Cyrillo, M., and Galvao, D. S.**

We have developed a new methodology to design conducting polymers with pre-specified properties. The methodology is based on the use of genetic algorithms (GAs) coupled to Negative Factor Counting technique. We present the results for a case study of polyanilines, one of the most important families of conducting polymers. The methodology proved to be able of generating automatic solutions for the problem of determining the optimum relative concentration for binary and ternary disordered polyaniline alloys exhibiting metallic properties. The methodology is completely general and can be used to design new classes of materials. (C) 2002 Elsevier Science B.V. All rights reserved

**Chemical Physics Letters 366[1-2], 170-175. 2002.**

**P122-02"Dipolar magnetic interactions among magnetic microwires".**

**Knobel, M., Sampaio, L. C., Sinnecker, E. H. C. P., Vargas, P., and Altbir, D.**

This paper presents a brief review of experiments and simulations on dipole-dipole interacting magnetic microwires that form a linear chain. In particular, recent studies on (a) amorphous Fe77.5Si7.5B15 and (b) granular Cu45Ni25Co29Mn1 microwires are discussed. Hysteresis loops were performed at room temperature for an array of N microwires (N = 1-5 for (a) and N = 1-100 for (b)) and compared with Monte Carlo simulations. In the case of amorphous soft magnetic materials (a), clear steps and plateaux on the demagnetization are visible, each step corresponding to the magnetization reversal of an individual wire. In the case of CuNiCoMn microwires (b), that exhibit a granular structure and a nearly superparamagnetic behavior when isolated, it was found that the coercivity abruptly changes from 20 to 700 Oe for N around 10. Novel Monte Carlo simulations are presented, providing useful insights about the effect of long-range interactions that account for the interesting observed magnetic behaviors. (C) 2002 Elsevier Science B.V. All rights reserved

**Journal of Magnetism and Magnetic Materials 249[1-2], 60-72. 2002.**

**P123-02"Experimental observation of high-field diamagnetic fluctuations in niobium".**

**Salem-Sugui, S., Friesen, M., Alvarenga, A. D., Gandra, F. G., Doria, M. M., and Schilling, O. F.**

We have performed a magnetic study of a bulk metallic sample of Nb with critical temperature T-c = 8.5 K. Magnetization versus temperature (M vs T) data obtained for fixed magnetic fields above 1 kOe show a superconducting transition which becomes broader as the field is increased. The data are interpreted in terms of the diamagnetic lowest Landau level (LLL) fluctuation theory. The scaling analysis gives values of the superconducting transition temperature T-c(H) consistent with H-c2(T). We search for universal three-dimensional LLL behavior by comparing scaling results for Nb and YBaCuO, but obtain no evidence for universality

**Physical Review B 66[13], art-134521. 2002.**

**P124-02"Exponential growth of particle number far from the parametric resonance".**

**de Melo, F. D. V. B., Brandenberger, R. H., and Maia, A.**

It is known that exponential particle creation can occur in situations which do not fall in the parametric resonance regime characterized by oscillations of the inflaton field about its minimum. Here we present a new analytical approach to exponential particle production which can occur when the inflaton is far from the minimum of its potential. Crucial for this effect is a term in the equation of motion which acts like a negative mass term, as occurs for tachyonic preheating and negative coupling particle production. Our techniques can be applied in models with a strong coupling between matter fields chi and the inflaton phi, or in some models in which the inflaton has a large amplitude of oscillation. On the other hand our analysis yields results which are quite model dependent. Although our analysis is general, in order to be clear we specialize, in this paper, to the model with interaction Lagrangian -gM(pl)phichi(2)

**International Journal of Modern Physics A 17[29], 4413-4418. 2002.**

**P125-02"Identifying relevant molecular descriptors related to carcinogenic activity of Polycyclic Aromatic Hydrocarbons (PAHs) using pattern recognition methods".**

**Coluci VR, Vendrame R, Braga RS, Galvao DS**

Polycyclic Aromatic Hydrocarbons (PAHs) constitute an important family of molecules capable of inducing chemical carcinogenesis. In this work we report structure-activity relationship (SAR) studies for 81 PAHs using the pattern-recognition methods Principal Component Analysis (PCA), Hierarchical Clustering Analysis (HCA) and Neural Networks (NN). The used molecular descriptors were obtained from the semiempirical Parametric Method 3 (PM3) calculations, We have developed a new procedure that is capable of identifying the PAHs' carcinogenic activity with an accuracy higher than 80%. PCA selected molecular descriptors that can be directly correlated with some models proposed to PAHs' metabolic activation mechanism leading to the formation of PAHs-DNA adducts. PCA, HCA and NN validate the energy separation between the highest occupied molecular orbital and its next lower level as a major descriptor defining the carcinogenic activity. This descriptor has been only recently discussed in the literature as one new possible universal parameter for defining the biological activity of several classes of compounds.

**JOURNAL OF CHEMICAL INFORMATION AND COMPUTER SCIENCES 42 (6): 1479-1489 NOV-DEC 2002**

**P126-02"Influence of interface mixing on the magnetic properties of Ni/Pt multilayers".**

**Frota-Pessoa, S., Klautau, A. B., and Legoas, S. B.**

Motivated by existing experimental data, we study here the influence of interface mixing on the magnetic behavior of Ni-6/Pt-5(111) multilayers. In the present ab initio calculations the mixing, restricted to the interface layers, was simulated by ordered two-dimensional Ni-Pt lattices. Two different degrees of mixing of the components at the interface were considered-namely, 25% and 50%. The perfect interface was also calculated and for some of the systems orbital moments were obtained. We find that interface mixing explains rather well the observed magnetic moment profile for Ni sites. But even with the inclusion of orbital contributions, the theoretical results tend to underestimate the induced moment at the Pt sites found experimentally

**Physical Review B 66[13], art-132416. 2002.**

**P127-02"Magnetic relaxation in nanocrystalline systems: linking Monte Carlo steps with time".**

**Vargas P, Knobel M, Altbir D**

The magnetic relaxation of a noninteracting two-dimensional ensemble of magnetic nanoparticles is simulated as a function of temperature using a Monte Carlo technique. By properly fitting the decay of magnetization using real parameters it is possible to make, at any finite temperature, a clear correspondence between Monte Carlo steps and time measured in seconds. The results allow one to visualize the intrinsic problems related to the simulation of nonequilibrium systems, and to understand the limits and range of validity of a particular system.

**ZEITSCHRIFT FUR METALLKUNDE 93 (10): 974-977 OCT 2002**

**P128-02"Magnetic structure of antiferromagnetic NdRhIn5".**

**Chang, S., Pagliuso, P. G., Bao, W., Gardner, J. S., Swainson, I. P., Sarrao, J. L., and Nakotte, H.**

The magnetic structure of antiferromagnetic NdRhIn5 has been determined using neutron
diffraction. It has a commensurate antiferromagnetic structure with a magnetic wave vector (1/2
01/2) below T-N=11 K. The staggered Nd moment at 1.6 K is 2.5(1)mu(B) aligned along the c axis.
This magnetic structure is closely related to the low-temperature magnetic structure of the cubic
parent compound NdIn3

**Physical Review B 66[13], art-132417. 2002.**

**P129-02"Magnetization plateaus and Luttinger liquid behavior in XXZ chains with superlattice structure".**

**Silva-Valencia J, Miranda E**

We study spin superlattices composed of a repeated pattern of two long spin-1/2 XXZ chains with different anisotropy parameters. They can be viewed as the limit of p-merized chains when the number of sites per cluster is very large. Magnetization plateaus are found, with magnetization values that depend On the relative sizes of the subchains, In certain regions of parameter space, the low-energy properties are described in terms of a Luttinger liquid superlattice parametrized by an effective velocity and an effective compactification radius.

**PHYSICAL REVIEW B 65 (2): art. no. 024443 . 2002**

**P130-02"MHD fluctuations and low energy solar neutrinos".**

**Guzzo, M. M., de Holanda, P. C., and Reggiani, N.**

We analyze here how future solar neutrino experiments could detect neutrino flux fluctuations due to magnetohydrodynamics (MHD) perturbations on the solar plasma. We state that if such time fluctuations are detected, this would provide a unique signature of the resonant spin-flavor precession (RSFP) mechanism as a solution to the solar neutrino problem

**European Physical Journal C 25[3], 459-464. 2002.**

**P131-02"Multiple ionization of atom clusters by intense soft X-rays from a free-electron laser".**

**Wabnitz, H., Bittner, L., de Castro, A. R. B., Dohrmann, R., Gurtler, P., Laarmann, T., Laasch, W., Schulz, J., Swiderski, A., von Haeften, K., Moller, T., Faatz, B., Fateev, A., Feldhaus, J., Gerth, C., Hahn, U., Saldin, E., Schneidmiller, E., Sytchev, K., Tiedtke, K., Treusch, R., and Yurkov, M.**

Intense radiation from lasers has opened up many new areas of research in physics and chemistry, and has revolutionized optical technology. So far, most work in the field of nonlinear processes has been restricted to infrared, visible and ultraviolet light(1), although progress in the development of X-ray lasers has been made recently(2). With the advent of a free-electron laser in the soft-X-ray regime below 100 nm wavelength(3), a new light source is now available for experiments with intense, short-wavelength radiation that could be used to obtain deeper insights into the structure of matter. Other free-electron sources with even shorter wavelengths are planned for the future. Here we present initial results from a study of the interaction of soft X-ray radiation, generated by a free-electron laser, with Xe atoms and clusters. We find that, whereas Xe atoms become only singly ionized by the absorption of single photons, absorption in clusters is strongly enhanced. On average, each atom in large clusters absorbs up to 400 eV, corresponding to 30 photons. We suggest that the clusters are heated up and electrons are emitted after acquiring sufficient energy. The clusters finally disintegrate completely by Coulomb explosion

**Nature 420[6915], 482-485. 2002.**

**P132-02"Multivector Dirac equation and Z(2)-gradings of Clifford algebras".**

**Mosna, R. A., Miralles, D., and Vaz, J.**

We generalize certain aspects of Hestenes's approach to Dirac theory to obtain multivector Dirac equations associated to a large class of representations of the gamma matrices. This is done by replacing the usual even/odd decomposition of the space-time algebra with more general Z(2)-gradings. Some examples are given and the chiral case, which is not addressed by the usual approach, is considered in detail. A Lagrangian formulation is briefly discussed. A relationship between this work and certain quaternionic models of the (usual) quantum mechanics is obtained. Finally, we discuss under what conditions the Hestenes's form can be recovered and we suggest a geometrical interpretation for the corresponding situation

**International Journal of Theoretical Physics 41[9], 1651-1671. 2002.**

**P133-02"Possible common ground for the metal-insulator phase transition in the rare Earth nickelates RNiO3 (R=Eu, Ho, Y)".**

**de la Cruz, F. P., Piamonteze, C., Massa, N. E., Salva, H., Alonso, J. A., Martinez-Lope, M. J., and Casais, M. T.**

We report on the infrared spectra of RNiO3 (R=Eu, Ho, Y). They provide evidence of phonon and insulating gap behavior and point to the monoclinic distortion at the metal-insulator (MI) transition as a feature for all RNiO3 (Rnot equalLa). We hypothesize that the intermediate paramagnetic phase (above T-N and below T-MI) in RNiO3 (R=Sm, Eu, Ho, Y) might be consequence of a self-doping effect, gradually triggering a phase segregation in electron-rich and electron-poor regions. This picture is concomitant to the temperature-dependent effect of octahedral tilting and distortion and self-trapped electrons in a polaronic medium

**Physical Review B 66[15], art-153104. 2002.**

**P134-02"Purification and growth of PbI2 crystals: Dependence of the radiation response on the PbI2 crystal purity".**

**Oliveira, I. B., Costa, F. E., Armelin, M. J., Cardoso, L. P., and Hamada, M. M.**

Lead iodide starting materials have been purified by a multipass; zone refining process. The effectiveness of the purification method on the material purity was determined by neutron activation analysis after three different purification passes numbers. A significant decrease of the impurities concentration was observed in function of the passes number. The purest material of the zone refined ingots, middle section, was used for crystal growth by Bridgman method. The results of the dark leakage current, the resistivity, and the response of the alpha and gamma radiations were strongly dependent on the purity of the crystal

**Ieee Transactions on Nuclear Science 49[4], 1968-1973. 2002.**

**P135-02"Quantifying the levitation picture of extended states in lattice models".**

**Pereira, A. L. C. and Schulz, P. A.**

The behavior of extended states is quantitatively analyzed for two-dimensional lattice models. A levitation picture is established for both white-noise and correlated disorder potentials. In a continuum limit window of the lattice models we find simple quantitative expressions for the extended states levitation, suggesting an underlying universal behavior. On the other hand, these results point out that the quantum Hall phase diagrams may be disorder dependent

**Physical Review B 66[15], art-155323. 2002.**

**P136-02"Role of group V exchange on the shape and size of InAs/InP self-assembled nanostructures".**

**Gutierrez HR, Cotta MA, Bortoleto JRR, de Carvalho MMG**

We have studied the influence of Group V overpressure on the final shape and size of InAs nanostructures grown on (001) InP substrates. The mechanisms leading to postgrowth modifications in the InAs nanostructures are discussed. The simultaneous action of Group V overpressure and stress field-produced by the InAs nanostructures-can induce strong material transport. The direction of this material net current depends on the type of Group V element used for the overpressure flux. In situ reflection high-energy electron diffraction, atomic force microscopy, and transmission electron microscopy measurements were used to characterize the transitions in morphology. Our results show that morphological studies considering the grown surface that do not take into account postgrowth processes can be misleading to understand the growth mechanisms governing the self-assembling process. (C) 2002 American Institute of Physics.

JOURNAL OF APPLIED PHYSICS 92 (12): 7523-7526 DEC 15 2002

**P137-02"Short-range interactions in a two-electron system: Energy levels and magnetic properties".**

**da Silva, L. G. G. V. and de Aguiar, M. A. M.**

The problem of two electrons in a square billiard interacting via a finite-range repulsive Yukawa potential and subjected to a constant magnetic field is considered. We compute the energy spectrum for both singlet and triplet states and for all symmetry classes as a function of the strength and range of the interaction and magnetic field. We show that the short-range nature of the potential suppresses the formation of "Wigner molecule" states for the ground state, even in the strong- interaction limit. The magnetic susceptibility chi(B) shows low-temperature paramagnetic peaks due to exchange induced singlet-triplet oscillations. The position, number, and intensity of these peaks depend on the range and strength of the interaction. The contribution of the interaction to the susceptibility displays paramagnetic and diamagnetic phases as a function of T

**Physical Review B 66[16], art-165309. 2002.**

**P138-02"Structure characterization and mechanism of growth of PbTe nanocrystals embedded in a silicate glass".**

**Craievich, A. F., Kellermann, G., Barbosa, L. C., and Alves, O. L.**

A nanocomposite consisting of PbTe nanocrystals embedded in a silicate glass was studied by small-angle x-ray scattering during the early stage of isothermal annealing at 793 K. A theoretical function based on a model of spherical PbTe nanocrystals surrounded by a Pb and Te depleted shell fits well to all experimental curves. The time dependences of the nanocrystal radius and size of the depleted shell agree with the prediction of the theory of nucleation and growth by the classical mechanism of atomic diffusion

**Physical Review Letters 89[23], art-235503. 2002.**

**P139-02"Study of the inhomogeneity of an alpha-particle source using Legendre polynomials".**

**Iunes, P. J., Bigazzi, G., Hadler, J. C., and Paulo, S. R.**

A mathematically simple methodology is presented for detecting spatial inhomogeneities of counts. The method is based on the use of Legendre polynomials. The methodology turned out to be appropriate also when applied to an alpha-particle source with a relatively small spatial inhomogeneity of alpha-particle emitters. For its simplicity its use may turn out to be advantageous also in other experiments also

**Journal of Radioanalytical and Nuclear Chemistry 254[2], 387-389. 2002.**

**P140-02"Testing the principle of equivalence by supernova neutrinos".**

**Guzzo, M. M., Nunokawa, H., and Tomas, R.**

We study the possible impact of the neutrino oscillation which could be induced by a tiny violation of equivalence principle (VEP) on the observation of neutrinos emitted from supernova driven by gravitational collapse. We show that using supernova neutrinos, one can probe very small values of VEP parameters, delta(tau) less than or similar to O(10(-31)) for massless or degenerated neutrinos and delta(tau) less than or similar to O(10(-16)) x (Deltam(2)/10(-5) eV(2)) for massive neutrinos. 

**Astroparticle Physics 18[3], 277-286. 2002.**

**P141-02"The effect of poly(ethylene glycol) on the activity and structure of glucose-6 phosphate dehydrogenase in solution".**

**Pancera, S. M., da Silva, L. H. M., Loh, W., Itri, R., Pessoa, A., and Petri, D. F. S.**

The effect of poly(ethylene glycol), PEG, on the enzymatic activity of glucose-6-phosphate dehydrogenase (G-6-PDH) in the oxidation of glucose-6-phosphate (G-6-P), using NADP+ as co- enzyme was investigated. The enzymatic activity was determined by means of spectrophotometry in three different media: pure Tris-HCl buffer, solution of PEG400 (20 wt.%) and of PEG4000 (20 wt.%), both in buffer. Comparing the enzymatic activity values measured in pure buffer with those in the polymer solutions, an increase in the enzymatic activity of 20% was observed in the presence of PEG400 as well as in PEG4000. Calorimetric studies indicated the absence of preferential interactions between G-6-PDH and PEG400 or PEG4000. Nevertheless, the interaction enthalpy, DeltaH(int), between NADP+ and PEG400 and PEG4000 amounted to -9.3 and -26.7 kJ/mol, respectively. Small angle X-ray scattering (SAXS) measurements were performed in a higher concentration range. Data analysis performed from SAXS curves by means of the intra-particle distance distribution function p (r) and Guinier plots yielded for G-6-PDH in pure buffer and PEG400 solutions radius of gyration, R-g, of about 70 Angstrom and in PEG4000 solutions, R-g of about 40 Angstrom. The latter has the same dimension as that found in the dimeric crystallographic structure of G-6- PDH, evidencing that G-6-PDH preserves its dimeric configuration in PEG4000 solution. On the contrary. different aggregates of G-6-PDH are formed in the presence of either buffer or PEG400. These findings show that the presence of PEG in solution can exert an effect on the enzyme structure and activity. 

**Colloids and Surfaces B-Biointerfaces 26[4], 291-300. 2002.**


# Abstracta

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