

# Abstracta

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**Trabalho Aceito para Publicação**

**A005-03 à A006-03**

**Artigo Aceito e Publicado em E-Print**

**E-print03-03**

**Trabalhos Publicados**

**P084-03 à P126-03**

## TRABALHOS ACEITOS PARA PUBLICAÇÃO

**A 005 - 03 "Entanglement dynamics in a two-mode nonlinear bosonic Hamiltonian".**

L. Sanz, R. M. Angelo, and K. Furuya

An Exactly soluble case of an interacting Hamiltonian of two bosonic modes is considered to study fundamental properties of the entanglement dynamics for a coupled nonlinear oscillators. Such an interaction is of physical importance, either in a two species Bose-Einstein condensed or in the case of two modes of electromagnetic field interacting in a Kerr media. The time-evolved state is obtained analytically for initial products of two. Fock and two coherent states, and the purification times of the subsystems determined. The possibility of dynamical generation of a quantum superposition state is discussed at such purification times. We also identify the existence of two regimes: the short time, phase spread regime where subsystems entropy rises monotonically and the self-interference regime where it oscillates and a purification phenomenon can be observed. Our results also show that the break time from the first regime to the second one becomes longer, as well as the purification and reversibility times, as the Planck's constant becomes much smaller than a typical action in phase space.

**Journal of Physics A: Mathem. and General 36[37], 9737-9754, 2003.**

**A 006 - 03 "Ordered quantization and the Ehrenfest time scale."**

R. M. Angelo, L. Sanz, and K. Furuya

We propose a prescription to quantize classical monomials in terms of symmetric and ordered expansions of noncommuting operators of a bosonic theory. As a direct application of such quantization rules, we quantize a classically time evolved function  $(q,p,t)$ , and calculate its expectation value in coherent states. The result can be expressed in terms of the application of a classical operator that performs a Gaussian smoothing of the original function evaluated at the center of the coherent state. This scheme produces a natural semiclassical expansion for the quantum expectation values at a short time scale. Moreover, since the classical Liouville evolution of a Gaussian probability density gives the same form for the classical statistical mean value, we can calculate the first-order correction in entirety from the associated classical time evolved function. This allows us to write a general expression for the Ehrenfest time in terms of the departure of the centroid of the quantum distribution from the classical trajectory, provided we start with an initially coherent state for each subsystem. In order to illustrate this approach, we have calculated analytically the Ehrenfest time of a model with  $N$ -coupled nonlinear oscillators with nonlinearity of even order.

**Physical Review E 68[1], 016206, 2003.**

## ARTIGO ACEITO E PUBLICADO EM E-PRINT

**E-print 03 - 03 "Entropy: Mystery and Controversy Plethora of Informational-Entropies and Unconventional Statistics".**

Luzzi, R., Vasconcellos, A. R., and Galvão Ramos, J.

Some general considerations on the notion of entropy in physics are presented. An attempt is made to clarify the question of the differentiation between physical entropy (the Clausius-Boltzmann one) and quantities called entropies associated to Information Theory, which are in fact generating functionals for the derivation of probability distributions and not thermodynamic functions of state. The role of them in the construction of the so-called Unconventional Statistical Mechanics, and the meaning and use of the latter, is discussed. Particular attention is given to the situation involving far-from-equilibrium systems.

**Statistical Mechanics 1, 213377, 2003.**

## TRABALHOS PUBLICADOS

**P 084 - 03 "Antihydrogen-hydrogen elastic scattering at thermal energies using an atomic-orbital technique"**

Sinha, P. K., Chaudhuri, P., and Ghosh, A. S.

In view of the recent interest in the trapping of antihydrogen atom (H) over bar, at very low temperatures, (H) over bar -H scattering has been investigated at low incident energies using a close-coupling model with the basis set  $(H) \text{ over bar } (1s, 2s, 2(p) \text{ over bar}) + H(1s, 2s, 2(p) \text{ over bar})$ . The predicted s-wave elastic phase shifts, scattering length, and effective range are in a good agreement with the other recent predictions of Jonsell and of Armour and Chamberlain. The results indicate that the atomic orbital expansion model is suitable to study the (H) over bar -H scattering at ultracold temperatures.

**Physical Review A 67[5], 052509. 2003.**

**P 085 - 03 "Ba Fe12019 thin film grown by an aqueous sol-gel process"**

Santos, J. V. A., Macedo, M. A., Cunha, F., Sasaki, J. M., and Duque, J. G. S.

In this communication we present a new sol-gel route to obtain high quality BaFe12O19 thin films. X-ray analysis confirmed the crystal structure with a crystal size of 32 nm. Atomic force microscopy images determined the film thickness to be around 250 nm and a roughness factor of less than 40 nm where the grain size averaged around 150 nm. SQUID magnetometer data shows a magnetic behavior similar to films grown by other techniques, namely, a coercive field ( $H_c = 4$  kOe), a normalized remanence close to 0.6 and saturation field of 15 kOe and  $M_s = 80$  emu/cm<sup>3</sup>.

**Microelectronics Journal 34[5-8], 565-567. 2003.**

**P 086 - 03 "Coupled channel formulation of the perturbed finite-temperature atomic random phase approximation: single channel approximation"**

Csanak, G., Kilcrease, D. P., and Meneses, G. D.

We present the spin and angular momentum analysis of the inhomogeneous coupled partial integro-differential equation formulation of the finite-temperature random phase approximation of an atom in a plasma. We demonstrate the cancellation of the direct and exchange self-interaction terms in the three-dimensional form of the equations. The direct self-interaction terms are also shown to cancel for each partial wave in the radial equations obtained from the spin and angular momentum analysis. We discuss how this inhomogeneous formulation avoids normalization difficulties encountered in our previous homogeneous eigenvalue formulation. Finally, the photoabsorption of the atom is given in terms of its polarizability.

**Journal of Quantitative Spectroscopy Radiative Transfer 81[1-4], 247-254. 2003.**

**P 087 - 03 "CP trajectory diagram - a tool for a pictorial representation of CP and matter effects in neutrino oscillations"**

Minakata, H. and Nunokawa, H.

We introduce a "CP trajectory diagram in bi-probability space" as a powerful tool for a pictorial representation of the genuine CP and the matter effects in neutrino oscillations. The existence of correlated ambiguity in the B is uncovered. The principles of tuning the beam energy for a determination of CP-violating phase  $\delta$  and the sign of  $\Delta m_{13}^2$  given baseline distance are proposed to resolve the ambiguity and to maximize the CP-odd effect. We finally point out, quite contrary to what is usually believed, that the ambiguity may be resolved with similar to 50% chance in the super-JHF experiment despite its relatively short baseline of 300 km.

**Nuclear Instruments & Methods in Physics Research Section A- Accelerators Spectrometers Detectors and Associated Equipment 503[1-2], 218-221. 2003.**

**P 088 - 03 "Cross-sectional Scanning Probe Microscopy of GaN-based p-n heterostructures".**

da Silva, M. I. N., Gonzalez, J. C., and Russell, P. E.

In this work, the structural and electrical properties of a GaN-based p-n heterostructure are studied using cross-sectional Atomic Force Microscopy, Friction Force Microscopy, Electrical Force Gradient Microscopy, and Surface Potential Microscopy. Using Atomic Force Microscopy and Friction Force Microscopy, we were able to identify and measure the thickness of the layers present in the heterostructures. The electrical conductivity type of the different layers as well as the p-n junction, and piezoelectric fields were identified and studied using Electric Force Gradient Microscopy and Surface Potential Microscopy.

**Microelectronics Journal 34[5-8], 571-573. 2003.**

**P 089 - 03 "Dimerization induced by the RKKY interaction"**

Xavier, J. C., Pereira, R. G., Miranda, E., and Affleck, I.

We report the presence of spin dimerization in the ground state of the one-dimensional Kondo lattice model at quarter filling. The emergence of this new phase of the Kondo lattice can be traced to the form of the RKKY interaction between the localized moments and provides the first example of dimerization induced indirectly by itinerant electrons. We propose this dimer ordering as the driving mechanism of the spin-Peierls phase observed in the quasi-one-dimensional organic compounds  $(\text{Per})_2(\text{M}(\text{mnt})_2)$  ( $\text{M}=\text{Pt}, \text{Pd}$ ). Moreover, this suggests that a richer phase diagram than the Doniach paradigm may be needed to accommodate the physics of heavy fermion materials.

**Physical Review Letters 90[24], art-247204. 2003.**

**P 090 - 03 "Effect of ion motion on rotating magnetic field current drive, The".**

Lifschitz, A. F., Farengo, R., and Clemente, R. A.

The effect of ion motion on rotating magnetic field (RMF) current drive in field reversed configurations is studied using a fully two-dimensional numerical code that solves the two fluid equations with massless electrons and constant uniform temperature. The ion momentum equation includes viscosity and collisions with neutrals, which remain fixed. The electrons are described with an Ohm's law that includes the Hall and pressure gradient terms. For full penetration of the RMF, ion spin-up due to collisions with electrons reduces the current drive efficiency and a large fraction of neutrals is needed to prevent the ions from acquiring high azimuthal velocities. For conditions that would result in incomplete penetration with the fixed ion model, ion rotation and variable density can facilitate the penetration of the RMF, thus increasing the efficiency. The rotation modifies the density profile and can trigger rotational instabilities.

**Plasma Physics and Controlled Fusion 45[6], 999-1012. 2003.**

**P 091 - 03 "Effects of a perturbative spike in open quantum dots: suppression of the conductance and discreet states imaging".**

Mendoza, M. and Schulz, P. A.

The ballistic transport of non-interacting electrons in open quantum dots (OQD) in the presence of a controllable perturbative spike is addressed. The changes in the conductance are systematically investigated as a function of the position of a perturbative potential spike moved along the systems. This analysis permits a clear identification of the quasi-bound and bound (localized) states and suppression of the conductance in the OQD. Moreover, a controllable way of tuning Fano resonances is proposed.

**Microelectronics Journal 34[5-8], 499-502. 2003.**

**P 092 - 03 "Electrical characterization of InGaN quantum well p-n heterostructures".**

Gonzalez, J. C., da Silva, M. I. N., Bunker, K. L., Batchelor, A. D., and Russell, P. E.

In this work, two methods for electrical characterization of InGaN quantum well p-n heterostructures at the nanometer level are presented. Cross-sectional Electrical Force Microscopy and High Resolution Electron Beam Induced Current (HR-EBIC) are used to study and identify regions of the cross-sectional surface of InGaN heterostructures with different types of electrical conductivity, the location of the InGaN quantum well, the location of the p-n junction, and the depletion layer. HR-EBIC was implemented in a Scanning Transmission Electron Microscope to take advantage of the high resolution chemical imaging capabilities of this microscope, such as Z- Contrast and Energy Dispersive X-ray Spectroscopy, and the small spread of the high energy electron beam in the electron transparent thin sample that allows electron beam induced current imaging with nanometer resolution.

**Microelectronics Journal 34[5-8], 455-457. 2003.**

**P 093 - 03 "Extrema bounds for the soft Pomeron intercept".**

Luna, E. G. S. and Menon, M. J.

By using an extended Regge parametrization and taking into account the discrepancies in the high-energy pp and (p) over barp total cross section data in both accelerator and cosmic-ray regions, we estimate extrema bounds for the soft Pomeron intercept. First we consider two ensembles of data with either the CDF or the E710 and E811 results for  $\sigma(\text{tot})(p)$  over  $\bar{p}p$  at 1.8 TeV, from which we obtain the bounds 1.102 and 1.081, respectively. These ensembles are then combined with the highest and lowest estimations for  $\sigma(\text{tot})(p)$  over  $\bar{p}p$  from cosmic-ray experiments (6-40 TeV), leading to the upper and lower bounds 1.109 and 1.082, respectively. The effects of simultaneous fits to  $\sigma(\text{tot})$  and  $\rho$ , individual fits to  $\sigma(\text{tot})$ , and the influence of the subtraction constant in the dispersion relations are also presented. Our global results favor the E710 and E811 data.

**Physics Letters B 565[1-4], 123-130. 2003.**

**P 094 - 03 "Formation dynamics of neutral and negatively charged excitons in double barrier resonant tunnelling structures".**

Vercik, A., Gobato, Y. G., and Brasil, M. M. P.

In this work we study the formation of neutral and negatively charged excitons in double barrier resonant tunnelling structures, by analyzing the dependence of photoluminescence emission on excitation intensity. At low excitation intensities, the negatively charged to neutral exciton intensity ratio depends linearly on the current, suggesting the validity of the concept of thermal equilibrium in these structures. At high excitation intensities, however, this model fails, and an abrupt transition occurs which is associated to the scattering between charged excitons and free carriers in the quantum well, which dissociates the trion.

**Microelectronics Journal 34[5-8], 659-661. 2003.**

**P 095 - 03 "Formation of quadrupolar vortices in ion-temperature-gradient modes".**

Qamar, A., Mirza, A. M., Murtaza, G., Vranjes, J., and Sakanaka, P. H.

Nonlinear equations which govern the dynamics of low-frequency ( $\omega \ll \omega_{ci}$ ), ion-temperature-gradient modes in the presence of equilibrium density, temperature, magnetic field, and electrostatic potential gradients are derived. For some specific profiles of the equilibrium flow velocity, number density, temperature, and magnetic field, new type of solutions in the form of quadrupole vortices are

found for a nondissipative plasma. The results can have relevance to the understanding of the salient features of anomalous ion thermal transport and coherent vortex structure formation in magnetically confined plasmas, such as in tokamaks.

**Physics of Plasmas 10[7], 2819-2823. 2003.**

**P 096 - 03 "Generalized coherent states for the double-well potential".**

**Novaes, M., de Aguiar, M. A. M., and Hornos, J. E. M.**

We construct generalized coherent states for the one-dimensional double-well potential and calculate their Mandel parameter, uncertainty relation and Wigner functions. The singularities of their autocorrelation function undergo bifurcations as the mean energy of the system is varied, and we analyse their structure. In the high-energy regime these states consist of a coherent superposition of two minimum-uncertainty Gaussians (they are Schrodinger catlike states).

**Journal of Physics A-Mathematical and General 36[21], 5773-5786. 2003.**

**P 097 - 03 "High resolution photoemission study of CdSe and CdSe/ZnS core-shell nanocrystals".**

**Borchert, H., Talapin, D. V., McGinley, C., Adam, S., Lobo, A., de Castro, A. R. B., Moller, T., and Weller, H.**

Colloidally prepared CdSe and CdSe/ZnS core-shell nanocrystals passivated with trioctylphosphine/trioctylphosphine oxide and hexadecylamine have been studied by photoelectron spectroscopy with tuneable synchrotron radiation. High-resolution spectra of the Se 3d level in CdSe nanocrystals indicate the bonding of organic ligands not only to surface Cd but also to surface Se atoms. The investigation of the CdSe/ZnS core-shell nanocrystals allows us to determine the average thickness of the ZnS shell and to study the interface between the two semiconductor nanomaterials. The photoemission spectra indicate a rather well ordered interface. No evidence for interfacial bonds other than Cd-S and Se-Zn is found.

**Journal of Chemical Physics 119[3], 1800-1807. 2003.**

**P 098 - 03 "Holographic phase-shift measurement during development of a fixed grating in lithium niobate crystals".**

**de Oliveira, I., Frejlich, J., Arizmendi, L., and Carrascosa, M.**

We report what is believed to be the first direct measurement of the grating phase-shift evolution during white-light illumination for the development of a fixed grating in an Fe-doped lithium niobate crystal. Stabilized holographic recording is shown to be essential for such measurements. Experimental data are in good agreement with theory and allow computation of the relevant material parameters for the sample under analysis. The results are of the utmost relevance for understanding the advantageous behavior of oxidized samples in hologram fixing.

**Optics Letters 28[12], 1040-1042. 2003.**

**P 099 - 03 "Hydrophobic surfaces probed by atomic force microscopy".**

**Teschke, O. and de Souza, E. F.**

We have measured the force acting on neutral tips as a function of distance to hydrophobic surfaces in aqueous solutions. The unusually large magnitude of this force is attributed to the electrostatic response of the aqueous fluid structure (hydration layer) at the interface. The local electric field in an interfacial region is a manifestation of the distribution of surface polar residues, and we have assumed that the polarization (hydration) of the hydrophobic surface immersed in water is predominantly driven by the direct

water binding. The simplest electrostatic description of the coupling between the interfacial polarization charges and the corresponding polarization charges of the solvent molecules is expressed here as the spatially variable dielectric permittivity  $\epsilon(\text{int})$ . The exchange of a volume of the interfacial region with  $\epsilon(\text{int})$  by a tip with a dielectric constant  $\epsilon(\text{tip})$  is responsible for the tip attraction. The variable dielectric permittivity profiles for the following interfaces were measured in order to clarify the origin of the long-range attractive forces: water/air, water/CTAB covered mica, and water/hydrophobic silicon.

**Langmuir 19[13], 5357-5365. 2003.**

**P 100 - 03 "Influence of the deposition method on the morphology and elemental composition of SnO<sub>2</sub> films for gas sensing: atomic force and X-ray photoemission spectroscopy analysis".**

**Bittencourt, C., Llobet, E., Silva, M. A. P., Landers, R., Nieto, L., Vicaro, K. O., Sueiras, J. E., Calderer, J., and Correig, X.**

The performance of metal oxide gas sensors is affected by their surface states, elemental composition, electronic and morphological structures. Films of tin oxide were deposited onto silicon substrates using reactive radio frequency sputtering and drop-coating. In order to understand how the deposition procedure affects the morphology of the films, a structural characterisation based on atomic force microscopy was performed. The differences in elemental composition were analysed by X-ray photoemission spectroscopy. For sensors deposited by sputtering, a granular morphology and the presence of stannic sub-oxide (SnO) was observed. Sensors deposited by drop coating had a granular morphology but no stannic sub-oxide was present. The sensitivity of the drop-coated sensors to ethanol was found to be up to five times higher than the one of sputtered sensors. This difference can be associated to the presence of the stannic sub-oxide, grain size and intergranular coupling.

**Sensors and Actuators B-Chemical 92[1-2], 67-72. 2003**

**P 101 - 03 "Inhomogeneous superconductivity in Bi<sub>2</sub>Sr<sub>2</sub>Ca<sub>1-x</sub>Pr<sub>x</sub>Cu<sub>2</sub>O<sub>8</sub>+ $\delta$ ".**

**dos Santos, C. A. M., Moehlecke, S., Kopelevich, Y., and Machado, A. S.**

We have studied Pr doping effect on the superconducting transition temperature onset  $T_C(x)$  in Bi<sub>2</sub>Sr<sub>2</sub>Ca<sub>1-x</sub>Pr<sub>x</sub>Cu<sub>2</sub>O<sub>8</sub>+ $\delta$  superconducting polycrystalline samples by means of both resistance  $R(T,x)$  and magnetization  $M(T,x)$  measurements. It is found that while the resistively determined  $T_{CR}(x)$  rapidly decreases with  $x$  for  $x > 0.4$ , the TCM approximate to 85 K obtained from magnetization measurements remains unchanged. We argue that the suppression of  $T_{CR}(x)$  is related to the reduction of the sample superconducting volume fraction which ultimately leads to disconnected superconducting clusters. Resistive behavior measured at different applied currents in a sample close to percolation threshold supports this discussion.

**Physica C-Superconductivity and Its Applications 390[1], 21-26. 2003.**

**P102-03 "Large nonlinear magnetoimpedance in amorphous Co<sub>80.89</sub>Fe<sub>4.38</sub>Si<sub>8.69</sub>B<sub>1.52</sub>Nb<sub>4.52</sub> fibers".**

**Duque, J. G. S., de Araujo, A. E. P., Knobel, M., Yelon, A., and Ciureanu, P.**

Fourier analysis of the nonlinear response of the impedance signal of amorphous Co<sub>80.89</sub>Fe<sub>4.38</sub>Si<sub>8.69</sub>B<sub>1.52</sub>Nb<sub>4.52</sub> fibers is presented. The harmonic components of the voltage signal present a strong asymmetry. A strong variation (around 1400%) of the second-harmonic signal ( $V_2(f)$ ) as a function of the applied magnetic field is observed. Nonlinear effects and the asymmetric behavior in harmonics can be associated with the anisotropies induced during the fabrication process. These results can lead to improvement of the performance of future

magnetoimpedance sensors.

**Applied Physics Letters 83[1], 99-101. 2003.**

**P 103 - 03 "Low-energy spin-wave excitations in the bilayered magnetic manganite  $\text{La}_2\text{2xSr1+2xMn2O7}$  ( $0.30 \leq x \leq 0.50$ )".**

**Martinho, H., Rettori, C., Huber, D. L., Mitchell, J. F., and Oseroff, S. B.**

We have studied the low-temperature behavior of the magnetization and specific heat of the bilayered perovskite system  $\text{La}_2\text{-2xSr1+2xMn2O7}$  for  $0.30 \leq x \leq 0.50$ . Our analysis reveals that below 30 K the temperature dependence of the magnetization of the ferromagnetic samples,  $x=0.30, 0.32, \text{ and } 0.36$ , in a field of 1 T can be interpreted in terms of the thermal excitations of a two-dimensional gas of ferromagnetic magnons. The specific heat in zero field for these samples, such as for the  $x=0.50$  antiferromagnetic one, is linear with temperature in the range of 1.8 K less than or equal to 10 K. This behavior can be also explained by the magnon gas model. By comparing specific heat measurements in zero field with those taken in a field of 9 T we are able to extract the lattice and electronic contributions and determine the in-plane exchange interactions. They are found to be in reasonable agreement with the values inferred from analysis of the magnetization data and also with the values reported by inelastic neutron scattering studies. In addition, we found that the electronic density of states obtained for the  $x=0.50$  sample is in agreement with previous band structure calculations.

**Physical Review B 67[21], art-214428. 2003**

**P 104 - 03 "Low-frequency spin dynamics in the  $\text{CeMn5}$  materials".**

**Curro, N. J., Sarrao, J. L., Thompson, J. D., Pagliuso, P. G., Kos, S., Abanov, A., and Pines, D.**

We measure the spin lattice relaxation of the planar  $\text{In}(1)$  nuclei in the  $\text{CeMn5}$  materials, extract quantitative information about the low energy spin dynamics of the lattice of Ce moments in both  $\text{CeRhIn5}$  and  $\text{CeCoIn5}$ , and identify a crossover in the normal state. Above a temperature  $T^*$  the Ce lattice exhibits "Kondo gas" behavior characterized by local fluctuations of independently screened moments; below  $T^*$  both systems exhibit a "Kondo liquid" regime in which interactions between the local moments contribute to the spin dynamics. Both the antiferromagnetic and superconducting ground states in these systems emerge from the Kondo liquid regime. Our analysis provides strong evidence for quantum criticality in  $\text{CeCoIn5}$ .

**Physical Review Letters 90[22], art-227202. 2003.**

**P 105 - 03 "Magnetic force images of nanomagnetic domains taken with platinum-coated tips".**

**Teschke, O., Kleinke, M. U., Dotto, M. E. R., Soares, D. M., Knobel, M., and de Souza, E. F.**

This article deals with magnetic force microscope images of nanosized domains in Co-coated films made by Pt-coated tips as well as micromagnetic images of data tracks written in recording media. Pt-coated tips have improved image delineation of the magnetic field distribution compared to images obtained by Co-coated hard magnetic tips. The force acting on Pt-coated tips in the magnetic field of the substrate was modeled assuming a paramagnetic tip. Due to the ferromagnetic nature of the interaction between the tip and substrate the spatial resolution of hard magnetic tips was shown to be inadequate to measure details of the features of nanosized domains. A comparison of the magnetic images made by Pt-coated tips with topographic images shows that magnetic domains resist thermal erasure at ambient temperature when they are formed of eight metallic grains.

**Journal of Applied Physics 94[1], 626-632. 2003.**

**P 106 - 03 "Magnetism in photopolymerized fullerenes".**

**Makarova, T. L., Han, K. H., Esquinazi, P., da Silva, R. R., Kopelevich, Y., Zakharova, I. B., and Sundqvist, B.**

The phototransformation of bulk C-60 and laser- and electron-beam treatment of C-60 films in air changes their magnetic properties. Nonlinear magnetization is observed only for samples irradiated in the presence of oxygen, while, in the case of pressure-polymerized C-60, oxygen adversely affects the magnetic properties. The contrasting roles of oxygen in these processes are discussed. Magnetic force microscopy shows that laser- and electron-beam irradiation of fullerene films produces magnetic images which are highly correlated with the topographic images.

**Carbon 41[8], 1575-1584. 2003.**

**P 107 - 03 "Measurements of long-range attractive forces between hydrophobic surfaces and atomic force microscopy tips".**

**Teschke, O. and de Souza, E. F.**

We have measured the force acting on neutral tips as function of distance to hydrophobic surfaces in aqueous solutions. The unusually large magnitude of this force is attributed to an electrostatic response of the aqueous fluid structure (hydration layer). The exchange of a volume of this region with a dielectric permittivity  $\epsilon(\text{int})$  by the tip with a dielectric constant  $\epsilon(\text{tip})$  is responsible for the tip attraction when it is immersed in the hydration layer. Hydrophobic hydration layers, characterized by a variable dielectric permittivity profile, have measured widths of similar to 4 and similar to 8 nm for hydrophobic silicon and CTAB monolayer covering mica surfaces, respectively.

**Chemical Physics Letters 375[5-6], 540-546. 2003.**

**P 108 - 03 "Note on dualities in Einstein's gravity in the presence of a non-minimally coupled scalar field, A".**

**Abramo, L. R., Brenig, L., Gunzig, E., and Saa, A.**

We show that the action of Einstein's gravity with a scalar field coupled in a generic way to spacetime curvature is invariant under a particular set of conformal transformations. These transformations relate dual theories for which the effective couplings of the theory are scaled uniformly. In the simplest case, this class of dualities reduces to the S-duality of low-energy effective action of string theory.

**Modern Physics Letters A 18[15], 1043-1051. 2003.**

**P 109 - 03 "Overlap optimization in semiconductor waveguides by wafer bonding".**

**Munoz, M. and Patel, N. B.**

In this work, we show that the use of a wafer-bonding technique, wherein an inverted half-waveguide structure is bonded on the upright half to form a complete waveguide, optimizes the overlap factor present in three-wave parametric interactions realized in  $(4) \text{ over } 3\text{m}$  semiconductor waveguides. These optimized waveguides can be used for efficient frequency-mixing devices which detect or emit infrared light.

**IEEE Journal of Quantum Electronics 39[6], 787-792. 2003.**

**P 110 - 03 "Phenomenology of 3+1 neutrino mass scheme".**

**Peres, O. L. G.**

We study the phenomenology of the 3 + 1-scheme is revisited in which the fourth (predominantly sterile) neutrino is isolated from a block of three flavour neutrinos by the mass gap  $\Delta m(\text{LSND})(2) \text{ similar to } (0.4-10) \text{ eV}(2)$ . The generic prediction of the scheme is the  $\nu(e)(-)$  and  $\nu(\mu)(-)$  disappearance probabilities at the level of present experimental bounds.

**P 111 - 03 "Photoionization and pseudopotentials".**

da Costa, R. F., Lima, M. A. P., and Ferreira, L. G.

Transferability of norm-conserving pseudopotentials to low-energy electron-molecule scattering processes has been very successful [Bettega, Phys. Rev. A 47, 1111 (1993)]. In this paper we discuss the possibility of using effective potentials in calculations of valence electrons photoionization cross sections. Through atomic targets, we illustrate that pseudopotentials can be optimized to give cross sections in good agreement with all-electron calculations. The present work represents a first step towards more elaborate computer programs for photoionization of molecular targets containing heavy atoms.

**Physical Review A 67[5], art-052706. 2003.**

**P 112 - 03 "Photoionization of CF<sub>4</sub> in the VUV region".**

Nascimento, E. M., Machado, L. E., Brescansin, L. M., and Lee, M. T.

We present calculated results of photoionization cross sections and photoelectron angular distributions for ionization out of the five outermost valence orbitals of CF<sub>4</sub> for photon energies ranging from near threshold to 55 eV. The Schwinger variational iterative method, using an exact static-exchange plus a model correlation-polarization potential, is applied to obtain the continuum photoelectron orbitals. The quantitative agreement between our calculated results and the experimental data is fair. Moreover, our study is capable of identifying most structures seen in experimental results for both cross sections and asymmetry parameters.

**Journal of Electron Spectroscopy and Related Phenomena 130[1-3], 101-109. 2003.**

**P 113 - 03 "Probing the LSND mass scale and four neutrino scenarios with a neutrino telescope".**

Nunokawa, H., Peres, O. L. G., and Funchal, R. Z.

We show in this Letter that the observation of the angular distribution of upward-going muons and cascade events induced by atmospheric neutrinos at the TeV energy scale, which can be performed by a kilometer-scale neutrino telescope, such as the IceCube detector, can be used to probe a large neutrino mass splitting,  $\Delta m_{21}^2$  similar to  $(0.5-2.0) \text{ eV}^2$ , implied by the LSND experiment and discriminate among four neutrino mass schemes. This is due to the fact that such a large mass scale can promote non-negligible  $\nu(\mu) \rightarrow \nu(e)$ ,  $\nu(\tau)/(\nu(\mu))$  over bar  $\rightarrow (\nu(e))$  over bar,  $(\nu(\tau))$  over bar conversions at these energies by the MSW effect as well as vacuum oscillation, unlike what is expected if all the neutrino mass splittings are small.

**Physics Letters B 562[3-4], 279-290. 2003**

**P 114 - 03 "Properties of fast submillimeter time structures during a large solar flare".**

Raulin, J. P., Kaufmann, P., de Castro, C. G. G., Pacini, A. A., Makhmutov, V. S., Levato, H., and Rovira, M.

We report properties of fast varying submillimeter emission during one of the strongest solar radio flares of solar cycle 23. Emission was obtained by the Solar Submillimeter-Wave Telescope at 212 and 405 GHz and compared with hard X-ray and gamma-ray counts up to few tens of MeV photon energy ranges. We employ different methods to detect and characterize flux density variations and find that during the impulsive phase of the event, the closer in time to the peak are, the higher the occurrence of the fastest and brightest time structures. The good comparison with hard X-ray and gamma-ray count rates indicates that fast submillimeter pulses are the signatures of primary energetic injections. The

characteristics of the fast spikes at 212 and 405 GHz, such as their flux density and localization, compared to those of the underlying slower impulsive component, also suggest that their nature is different.

**Astrophysical Journal 592[1], 580-589. 2003.**

**P 115 - 03 "Respiratory pattern changes in elderly yoga practitioners".**

De Barros, R. M. L., Leite, M. R. R., Brenzikofer, R., Filho, E. C. L., Figueroa, P. J., and Iwanowicz, J. B.

The purpose of this research was to study yoga induced thoracoabdominal motion pattern changes during breathing in elderly female subjects. A group of 11 elderly volunteers (mean age: 66.7 +/- 6.4yrs) who had been practising yoga (YG) regularly for over 3yrs was compared to a control group (CG) of 11 non-sedentary volunteers (mean age: 65.7 +/- 7.0yrs). Each subject had 14 markers fixed directly to the skin of the anterior trunk surface and performed twelve vital capacity (VC) manoeuvres in an upright position. A kinematical analysis system was used to measure the trajectory of these markers. Bivariate interpolation function and smooth surface fittings for irregularly distributed data were applied to the set of reconstructed points and thus accurate representation of the trunk surface was obtained as a function of time. Total and partial areas of the surface and a temporal evolution of these measures were calculated. The correlation coefficients for the thorax area (TA) and the abdomen area (AA) of the anterior part of the trunk were used as measures related to the subject's respiratory pattern. No significant differences ( $p > 0.05$ ) were found regarding age, height, weight, mean TA and mean AA in the YG and CG. Highly significant differences were obtained ( $p < 0.001$ ) with regard to the mean values of YG and CG (in parenthesis), breathing frequency, root mean square deviation of TA and AA and in the z-transformed correlation coefficient used to measure the respiratory patterns. The results indicate that yoga techniques may lead to the formation of specific respiratory patterns as well as to reduced breathing frequency and increased breathing amplitude.

**Journal of Human Movement Studies 44[5], 387-400. 2003.**

**P 116 - 03 "Silicon neighborhood across the a-Si : H to  $\mu$ c-Si transition by X-ray absorption spectroscopy (XAS), The".**

Tessler, L. R., Wang, Q., and Branz, H. M.

We report a synchrotron X-ray absorption spectroscopy study of the average neighborhood of Si near the transition from a-Si:H to  $\mu$ c-Si on wedge-shaped samples prepared by hot-wire CVD in a chamber using a movable shutter. The thickness of the wedge varies from 30 to 160 nm. Nucleation of  $\mu$ c-Si occurs at a critical thickness of approximately 100 nm. X-Ray absorption was measured at the Si K-edge (1.84 keV) by total electron photoemission yield. The absorption oscillations in the EXAFS region are very similar to all along the wedge. Analysis indicates an average tetrahedral first neighbor shell with radial disorder decreasing with crystallization. In the near-edge (XANES) region multiple scattering effects appear at the onset of crystallinity. Unlike single crystal silicon, these effects involve only double scattering, within the first neighbor shell, indicating an ill-formed second shell in  $\mu$ c-Si.

**Thin Solid Films 430[1-2], 83-86. 2003.**

**P 117 - 03 "Solving the boundary value problem for finite Kirchhoff rods"**

da Fonseca, A. F. and de Aguiar, M. A. M.

The Kirchhoff model describes the statics and dynamics of thin rods within the approximations of the linear elasticity theory. In this paper we develop a method, based on a shooting technique, to find equilibrium configurations of finite rods subjected to boundary conditions and given load parameters. The method consists in making a series of small changes on a trial solution satisfying the Kirchhoff equations but not necessarily the boundary conditions. By linearizing the

differential equations around the trial solution we are able to push its end point to the desired. position, step by step. The method is also useful to obtain configurations of rods with fixed end points but different mechanical parameters, such as tension, components of the moment or inhomogeneities.

**Physica D-Nonlinear Phenomena 181[1-2], 53-69. 2003.**

**P 118 - 03 "Spatially resolved electrical properties of InAs/InP quantum dots and wires".**

**Vicaro, K. O., Cotta, M. A., Gutierrez, H. R., and Bortoleto, J. R. R.**

In this paper the electrical properties of InAs/InP nanostructures (wires and dots) were investigated using Kelvin probe electrostatic force microscopy and conductive atomic force microscopy techniques. Surface potential measurements were strongly affected by the presence of the thin InAs film at the top surface of the undoped InP buffer layer. These results and the electrical images suggest the suppression of the surface depletion region due to electron accumulation in InAs wires and dots. I-V spectroscopy shows the formation of a Schottky-type junction between the metal-coated Si tip and the semiconductor surface exposed to air. Larger conductances and different threshold voltages for current onset for the two types of nanostructure analysed here can be related to the particular electronic structure of InAs wires and dots.

**Nanotechnology 14[5], 509-514. 2003.**

**P 119 - 03 "Spin-orbit induced backflow in neutron matter with auxiliary field diffusion Monte Carlo method".**

**Brualla, L., Fantoni, S., Sarsa, A., Schmidt, K. E., and Vitiello, S. A.**

The energy per particle of zero-temperature neutron matter is investigated, with particular emphasis on the role of the L.S interaction. An analysis of the importance of explicit spin-orbit correlations in the description of the system is carried out by the auxiliary field diffusion Monte Carlo method. The improved nodal structure of the guiding function, constructed by explicitly considering these correlations, lowers the energy. The proposed spin-backflow orbitals can also be conveniently used in the Green's function Monte Carlo calculations of light nuclei.

**Physical Review C 67[6], art-065806. 2003.**

**P 120 - 03 "Strain-induced ordering in In<sub>x</sub>Ga<sub>1-x</sub>N alloys".**

**Teles, L. K., Ferreira, L. G., Leite, J. R., Scolfaro, L. M. R., Kharchenko, A., Husberg, O., As, D. J., Schikora, D., and Lischka, K.**

The energetics and thermodynamic properties of cubic (c-)In<sub>x</sub>Ga<sub>1-x</sub>N alloys are investigated by combining first-principles total energy calculations, a concentration-dependent cluster-based model, and Monte Carlo simulations. The search for the ground-state energies leads to the conclusion that biaxial strain suppresses phase separation, and acts as a driving force for chemical ordering in c-In<sub>x</sub>Ga<sub>1-x</sub>N alloys. Ordered superlattice structures, with composition x congruent to 0.5 and stable up to T=1000 K, arises as the relevant thermodynamic property of the strained alloy. We suggest that the In-rich phases recently observed by us in c-GaN/In<sub>x</sub>Ga<sub>1-x</sub>N/GaN double heterostructures are ordered domains formed in the alloy layers due to biaxial strain.

**Applied Physics Letters 82[24], 4274-4276. 2003.**

**P 121 - 03 "Structural characterization of TiO<sub>2</sub>/TiN<sub>x</sub>O<sub>y</sub> (delta-doping) heterostructures on (110)TiO substrates".**

**Chiaramonte, T., Cardoso, L. P., Gelamo, R. V., Fabreguette, F., Sacilotti, M., de Lucas, M. C. M., Imhoff, L., Bourgeois, S., Kihn, Y., and Casanove, M. J.**

TiO<sub>2</sub>/TiN<sub>x</sub>O<sub>y</sub> delta-doping structures were grown on the top of

(1 1 0)TiO<sub>2</sub> rutile substrates by low pressure metal-organic vapor phase epitaxy (LP-MOVPE) technique at 750 degrees C. The samples were analyzed by high resolution transmission electron microscopy (HRTEM), electron energy loss spectroscopy (EELS) and X-ray diffraction techniques (rocking curves and phi-scans). The presence of satellites in the (1 1 0)TiO<sub>2</sub> rocking curve revealed the epitaxial growth of 10 period delta-doping structures. The thickness of the TiO<sub>2</sub> layers, 84 nm, was deduced from the satellites period. HRTEM observations showed around 1.5 nm thick delta-doping layers, where the presence of nitrogen was detected by EELS. The analysis of the Bragg surface diffraction peaks observed in the phi-scans points to an almost negligible strain in this sample which was confirmed by substrate curvature radius measurements.

**Applied Surface Science 212, 661-666. 2003.**

**P 122 - 03 Study of oxygen influence in the production of single-wall carbon nanotubes obtained by arc method using Ni and Y catalyst.**

**Montoro LA, Luengo CA, Rosolen JM, Cazzanelli E, Mariotto G**

Single-wall carbon nanotubes were produced by arc method (He atmosphere) using Ni/Y<sub>2</sub>O<sub>3</sub> and NiO/Y<sub>2</sub>O<sub>3</sub> catalysts. The samples obtained by both the catalysts were collected in two regions of reactor: collar and walls zones. The raw material was also submitted to ultrasonic and filtration treatments using a surfactant aqueous solutions of sodium dodecyl sulphate. Raman scattering and transmission electron microscopies were used as characterisation tools. The distribution of carbon nanotube (CNT) content depends on the zone from which samples are collected. In particular the highest CNT content is found in specimens coming from the collar zone when NiO/Y<sub>2</sub>O<sub>3</sub> catalyst is employed. In fact, the presence of NiO in the catalyst seems to favour the CNT yield, despite of the consistent amount of the carbon impurities (amorphous carbon and graphite) still present in the raw material. Finally, the surfactant treatment effectively reduces the carbon impurities in the residue thus allowing for an appreciable separation of the CNT component. (C) 2003 Elsevier Science B.V. All rights reserved.

**DIAMOND AND RELATED MATERIALS 12 (3-7): 846-850 MAR-JUL 2003**

**P 123 - 03 "Temperature effects on dislocation core energies in silicon and germanium"**

**Miranda, C. R., Nunes, R. W., and Antonelli, A.**

Temperature effects on the energetics of the 90degrees partial dislocation in silicon and germanium are investigated, using nonequilibrium methods to estimate free energies, coupled with Monte Carlo simulations. Atomic interactions are described by Tersoff and environment-dependent interatomic potentials. Our results indicate that the vibrational entropy has the effect of increasing the difference in free energy between the two possible reconstructions of the 90degrees partial, namely, the single-period and the double-period geometries. This effect further increases the energetic stability of the double-period reconstruction at high temperatures. The results also indicate that anharmonic effects may play an important role in determining the structural properties of these defects in the high-temperature regime.

**Physical Review B 67[23], art-235201. 2003.**

**P 124 - 03 "Thermomechanical properties of the amorphous carbon nitride thin films".**

**Champi, A., Lacerda, R. G., and Marques, F. C.**

In this work we investigated thermomechanical properties of carbon nitride thin films. The thermal expansion coefficient and the elastic constants were studied as a function of the nitrogen concentration. Drastic changes of the film structure were observed as a result of the nitrogen incorporation, varied from 0 to 7%. It was observed that the thermal expansion coefficient has a significant increase from about 2 to 9 x 10<sup>-6</sup>

K-1. This results were attributed to the increase in the concentrations of sp(2) sites and clusters sizes.

**Microelectronics Journal 34[5-8], 553-555. 2003.**

**P 125 - 03 "two-gap superconductivity in MgB<sub>2</sub>".**

**Ghosh, A.**

We study the superconductivity in MgB<sub>2</sub> using a tight binding model to investigate the doping dependence of the order parameter and the critical temperature. We consider both the anisotropic and the isotropic s-wave pairing to study the coexistence of the two gaps. A good agreement between the existing experiments and our theoretical curves is observed. The temperature dependence of order parameter, specific heat and penetration depth at half filling are also demonstrated and are found to be in accord with the available experimental predictions

**International Journal of Modern Physics B 17[13], 2589-2598. 2003.**

**P 126 - 03 "Vertical stacks of InAs quantum wires in an InP matrix".**

**Gutierrez, H. R., Cotta, M. A., and de Carvalho, M. M. G.**

In this work, multilayered films-consisting of layers of self-assembled InAs quantum wires separated by InP spacers-were deposited on (0 0 1) InP substrates. We studied the vertical alignment of the nanostructures by using cross-section transmission electron microscopy (XTEM). A clear relation between the geometry of the wire cross-section and the stacking angles was observed. For asymmetric wires the stacking angle with respect to the growing direction is larger. Moreover, XTEM shows that the strain field generated by two nanowires can induce the nucleation of a unique wider nanowire in the subsequent InAs layer. Similarly to quantum-dot multilayers systems, this mechanism could produce uniform width distribution for the self-assembled nanowires.

**Journal of Crystal Growth 254[1-2], 1-5. 2003.**

# Abstracta

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