I WORKSHOP do Programa de Pós-Graduação em Física

LIVRO DE RESUMOS

21 a 23 de Março de 2018

I WORKSHOP do Programa de Pós-Graduação em Física

LIVRO DE RESUMOS

UFPR EXATAS

UFPR 105 ANOS DE ORGULHO

UFPR FÍSICA

CNPq
Conselho Nacional de Desenvolvimento Científico e Tecnológico

CAPES

FUNDAÇÃO ARAUCÁRIA
Apoio ao Desenvolvimento Científico e Tecnológico do Paraná

Cronograma do IWPPGF			
	Dia 21/03	Dia 22/03	Dia 23/03
08h30	Abertura	-	-
09h00	Palestra 1	Apresentações orais 3	Apresentações orais 5
10h00	Intervalo	Intervalo	Intervalo
10h30	Apresentações orais 1	Apresentações orais 4	Apresentações orais 6
12h00	Almoço	Almoço	Almoço
14h00	Apresentações orais 2	Palestra 2	Palestra 3
15h00	Intervalo	Intervalo	Intervalo
15h30	Apresentações de pôsteres 1	Apresentações de pôsteres 2	Plenária de encerramento do evento
17h00	Encerramento do dia	Confraternização Local: ASUFEPAR	

Palestra 1: Prof. Dr. Ricardo Luiz Viana – Departamento de Física da UFPR.

Tema: Breve histórico do Programa de Pós-Graduação em Física da UFPR.

Palestra 2: Prof. Dr. Jan-Michel Rost – Max Planck Institute for the Physics of Complex Systems, Dresden, Alemanha.

Tema: Rydberg molecular systems: From antiprotonic Helium to Trilobites in a dense gas.

Palestra 3: Prof. Dr. André Luiz Felix Rodacki – Coordenador de Programas de Pós-Graduação – *Stricto sensu* da UFPR.

Tema: A Pós-Graduação na UFPR.

Apresentações orais 1 (21/03)*		
Manhã	10h30	Prof. Dr. Ricardo Viana
	10h50	Prof. Ivo Hummelgen
	11h10	Prof. Dr. Felix Sharipov
	11h30	Prof. Dr. Wilson Marques Jr.
Apresentações orais 2 (21/03)*		
Tarde	14h00	Cesar Augusto
	14h20	Roberto Budzinski
	14h40	Andressa Toppel

* Tempo das apresentações orais: 20 minutos.

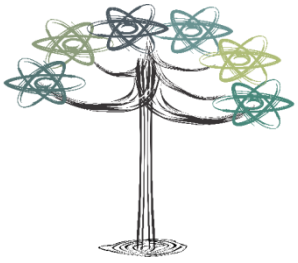
Manhã	**Apresentações orais 3 (22/03)***	
	09h00	Leandro Cesar Mehret
	09h20	Karla Weber
	09h40	Bruno Boaretto
	Apresentações orais 4 (22/03)*	
	10h30	Prof. Dr. Marcio Bettega
	10h50	Prof. Dr. Marcus Beims
	11h10	Prof. Dr. Dante Mosca
	11h30	Profª. Drª. Lucimara S. Roman

* Tempo das apresentações orais: 20 minutos.

Manhã	**Apresentações orais 5 (23/03)***	
	09h00	Thales Silva
	09h20	Raul de Palma Aristides
	09h40	Guilherme Alexandre Emidio
	Apresentações orais 6 (23/03)*	
	10h30	Aron Luiz Oliveira dos Santos
	10h50	Prof. Dr. Marcos Gomes
	11h10	Prof. Dr. Renato M. Angelo
	11h30	Prof. Dr. Miguel Abbate

* Tempo das apresentações orais: 20 minutos.

Apresentações dos pôsteres 1 (21/03)		Apresentações dos pôsteres 2 (22/03)	
1	Carlos Fábio de Oliveira Mendes	1	Viviane Stoeberl
2	Leandro Benatto	2	Fernanda Coff Dias
3	Maiara de Jesus Bassi	3	Sidney Tiago da Silva
4	Aluizio Jose Salvador	4	Greici Gubert
5	Nicholas Figueiredo Prestes	5	Karlisson R. de Almeida Sousa
6	Deize Corradi Grodniski	6	Ronei Cardoso de Oliveira
7	Adam Luiz de Azevedo	7	Mylena Hortz Ribas
8	Adriane Reis	8	Flavio Prebianca
9	Samuel Domenech	9	Elberth Manfron Schiefer
10	Rafael Marques da Silva	10	Anne Beatriz Rocha Abreu
11	Giseli Maria Moreira	11	Arlans Juan Smokovicz de Lara
12	Flávio Roberto Rusch	12	Marcelo Henrique Penteado
13	Edjan Alves da Silva	13	Matheus Bacigalupo Kistaki
14	Victor Juan Benites	14	Pedro Ruas Dieguez
15	Adriano de Souza Silva	15	Elton Moura
16	Mateus Peres Genaro	16	Vitor Cardoso Castro Brasil
17	Alfredo Enrique Macias Medri	17	Letícia da Silva Maioli
18	Valber da Silva Gomes	18	Ravel de Moraes Telles Araujo



I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA

21 a 23 de Março de 2018

An investigation of Bethe Ansatz solution for two distinct interacting particles in a 1D region

Azevedo, A.L.[1], Luz, M. G. E. [2]

[1] *UFPR*

[2] *UFPR*

Abstract: Classical integrable systems with short-range potential can be described by a finite superposition of plane waves in Quantum Mechanics (Bethe Ansatz). In general, in these physical systems, the particles are identical, as is the case of the problem of N interacting bosons by Dirac delta potential and confined in a 1D box. Of course, this is true for 2 particles (bosons). But, in classical description, the only integrable system for particles of different masses is that where the mass ratio equal to 3. We then investigate whether it is possible to construct a Bethe Ansatz solution for this particular case. This analysis allowed us to obtain the solution when interaction potential between the particles is infinite, and also for an interesting case of a kite-shaped billiard.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Dynamical properties of a neuronal network described by coupled Rulkov maps

A. S. Reis[1], R. L. Viana[1].

[1] *Universidade Federal do Paraná – Departamento de Física.*

The nervous system is divided into two parts that correspond to the central nervous system (CNS) and peripheral nervous system (PNS). Our brain is a vital organ that controls all the basic functions o four body through electrical impulses. These electrical impulses are transmitted by our neurons, which by you own definition are the eletrically excitable cells that process and transmit information through electrical and chemical connections between other neurons.

In this work we will present a study of a neural networks made from the Rulkov map. The Rulkov map has long been use as a model that allows us to understand the (temporal) dynamics of a neural network. This map show us two time scales (one fast and the onter one slow) that are quit similar to those found in the electrical shots between the neurons.

$$x_{n+1} = \frac{\alpha}{1 + x_n^2} + y_n$$

$$y_{n+1} = y_n - \sigma(x_n - \rho)$$

Here x represents the fast variable, which can be associated to neuron membrane potential and the y is the slow variable. We must say that the y variable doesn't have any biological meaning which is just the opposite of the variable x. It is importante to note that α and ρ give us diferente dynamical states of the neuron like resting, spking and chaotic bursts.

The neural network model described here presentes small world property (high clustering coefficient and shortest path length). A phase synchronization as these abnormal rhythms in the brain can cause Parkinson's disease and essential tremor.

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21 a 23 de Março de 2018

Chemical sensors based on Cu_3N nanoparticles for distinction of beer made with malted barley from beer prepared with other malted cereals: A preliminary study

Adriano de S. Silva[1], Rafael Rodrigues[1], Rudo Sithole[2], Siziwe Gqoba[2], Makwena J. Moloto[2], Juanita van Wyk[2], Nosipho Moloto[2], Ivo A. Hümmelgen[1]

[1] *Departamento de Física, Universidade Federal do Paraná, Curitiba – Paraná, Brazil.*

[2] *School of Chemistry, Molecular Sciences Institute, University of the Witwatersrand, Johannesburg – Gauteng, South Africa.*

Copper nitride, Cu_3N, is a semiconductor with an indirect band gap of 1.04 eV and direct band gap between 0.7 and 1.12 eV. Cu_3N has a primitive open anti-rhenium trioxide cubic structure with nitrogen atoms occupying the corners of the cube and a cooper atom found in-between two consecutive nitrogen atoms. The face centers and the body of the cube are not occupied in pure copper nitride and this leaves void interstitial sites that can be occupied by either copper, nitrogen or other foreign atoms. The occupation of these sites alters the optical and electrical properties and has been reported to result in the transition from a semiconductor to a conductor. Copper nitride nanoparticles were synthesized using $C_{16}H_{22}N_4Cu$ as precursor and characterized by X-ray diffraction (XRD), X-ray photoelectron spectroscopy (XPS), transmission electron microscopy (TEM), ultraviolet-visible spectroscopy (UV-vis) and photoluminescence spectroscopy (PL). After characterization, Cu_3N nanoparticles were applied as active monolayer and multilayers in three nonspecific chemical sensors set for distinction of two distinct beers, as a preliminary study. In future, the study will be extended aiming the development of a procedure that allows the distinction of beer prepared from malted barley from beer prepared from other malted cereals. Impedance spectroscopy (IS) measurements were performed in LCR meter to evaluate the electrical behavior of the samples. The data obtained from impedance spectroscopy measurements were analyzed using a pattern recognition method named tristimulus, allowing distinction between both types of samples.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Synthesis and characterization of Polypyrrole@α-Al_2O_3 and Polypyrrole@CeO_2 core-shell hybrid nanocomposites

Adriano de S. Silva[1,2], Edgar A. Sanches[2]

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[2] *Departamento de Física, Universidade Federal do Amazonas, Manaus – Amazonas, Brazil.*

Polypyrrole and Polypyrrole@α-Al_2O_3, Polypyrrole@CeO_2 core-shell hybrid nanocomposites were synthesized free of acids by *in situ* polymerization and characterized by x-ray diffraction (XRD), scanning electron microscopy (SEM), differential scanning calorimetry (DSC) and DC electrical conductivity measurements. XRD pattern of PPy reveled a semi crystalline structure. The Le Bail method was performed using the XRD pattern of PPy and allowed of the unit cell parameters: $P21/c$, $a=9.0173\,\AA$, $b=7.1641\,\AA$, $c=6.4184\,\AA$, $\alpha=90°$, $\beta=117.7°$ and $\gamma=90°$; which is composed by a dimeric molecule disposed along the [001] direction. A cauliflower morphology was observed in PPy, which consists of incomplete spheres forming nanoparticles clusters, however core-shell morphology was verified in the hybrid nanocomposites consisting of a thin layer of polymeric reinforcement disposed over the metal oxides matrices. DSC measurements allowed verifying the hydrophobic behavior of the inorganic phase, promoting the repulsion of the internal water molecules out from the polymer phase. Then the initial decomposition temperature of the nanocomposites has become smaller. The PPy DC electrical conductivity is lower than the hybrid nanocomposites and may be related with the absence of hydration water in nanocomposites and also to the surface conductivity due to the thin polymer layer. PPy@α-Al_2O_3 and PPy@CeO_2 hybrid nanocomposites presented DC electrical conductivity 80% higher when compared to the as-synthesized PPy. Thus, the aim of this work was to characterize structural and morphologically the pure PPy as well PPy@α-Al_2O_3 and PPy@CeO_2 hybrid nanocomposites and correlate these results with the DC electrical conductivity measurements.

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21 a 23 de Março de 2018

Probabilistic approach to determining temperature sets for simulated tempering methods

A.E. Macias-Medri[1], M.G.E. da Luz[1], Carlos E. Fiore[2].

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[2] *Instituto de Física, Universidad de São Paulo, CP 66318, 05315-970 São Paulo-SP, Brazil.*

It is presented a probabilistic equilibrium scheme to computing the temperature replicates of simulated tempering simulations. The simulated tempering based on monte carlo methods allows to predict first order phase transitions through temperature changes with pre-fixed values (replicates). Over the run time and in each monte carlo step, the changes are accepted probabilistically by free energy differences. The values of these differences are previously calculated by using simulated annealing techniques and matrix transfer methods. The choose of the appropriate replicates can mean efficient in the sense of tunneling and convergence of macroscopic measures. Currently, the technique of direct estimation of interchange frequencies between replicates [Comput.Phys.Comm. 185 (2014) 2046] is the more efficient, however, this implies perform a set of simulations with few iterations that it can be sensitive to specific physical models. In this sense, in this work we propose to calculate the interchange frequencies by direct relation with transition probabilities of the steady state. This model is implemented to new simulated tempering runs and our results are compared with traditional techniques.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Chemical disorder and functionalities of Ni_2MnGa and Mn_2NiGa alloys

Aluizio José Salvador, Dante Homero Mosca Jr.

Laboratório de Superfícies e Interfaces

Universidade Federal do Paraná - UFPR.

The aim of this Master of Science work is investigate the chemical disorder in thin films of Ni_2MnGa and Mn_2NiGa grown by molecular beam epitaxy on crystalline substrates. The chemical disorder is a defect due to the probabilistic mutual exchange of atoms in the crystalline structure of the alloy. Chemical and structural disorder can be separated through X-ray and electron diffraction measurements whereas, the average stoichiometry can be determined by photoelectron spectroscopy analyses. Crystalline and highly textured thin films of Ni_2MnGa and Mn_2NiGa are currently grown by MBE at the Group of Films and Magnetic Nanostructures of UFPR. These alloys are ferromagnetic with rather distinct magnetic moments on Ni and Mn sites and both alloys exhibit the magnetic shape memory (MSM) effect. In the thin film geometry with nanometric thickness MSM effect, total magnetic moment per formula unit and lattice parameters become strongly dependent on the structural and chemical disorder. Residual strain commonly induced in the films due to the lattice mismatch between and substrate in the epitaxial relationships can be relaxed by thermal cycling and post-annealing procedures. However, intrinsic antisite disorder is quite difficult to mitigate in these Heusler alloys (nominally X_2YZ), which adopt the $L2_1$-type crystal structure consisting of four equivalent interpenetrating face centered cubic structures (X_I, X_{II}, Y and Z, where I and II denote two equivalent sites). The stoichiometry of the X_2YZ alloy films and the chemical state of elements in the alloying is determined by in situ X-ray photoelectron spectroscopy analyses. Ex-situ X-ray diffraction experiments are used to probe the chemical disorder by comparing the relative intensity of Bragg reflections corresponding to the crystalline planes of families (nnn), (0nn) and (n00), considering the atomic and structure factors for perfectly ordered alloys structurally and chemically. Essentially, the modeling will consist in establishing statistical relation between the lattice site occupations by the three possible atoms that better reproduce the ratio of diffraction peak intensities. Eventually, magnetization measurements will also be performed using a Physical Property Measurement System (PPMS Evercool II) in order to evaluate the changes in the saturation magnetization of the thin films.

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DEVELOPMENT OF EPOXY RESIN BASED ORGANIC SINGLE AND MULTI LAYER MEMORY DEVICES.

Andressa Toppel [1], Celso de Araujo Duarte [2],

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[2] *Departamento de Física, Universidade Federal do Paraná, CP 19044, 81531-990, Curitiba (PR), Brazil.*

This study presents a review about organic memory devices like WORM (Write Once Read Many times) having as active layer thin films of epoxy resin nanocomposites and single-layer or multi-layer carbon nanostructures. Epoxy resin was used as polymer matrix for its many advantages allowing the possibility of using the same component in the fabrication of the active layer and the encapsulation simultaneously (consisting of the so-called "AW1" technique previously created in our research group [1]). In order to confer bistability to the resin (which in itself is a great insulator) and to enable its use in the development of the WORM memories, a controlled fraction of conductive carbon nanostructures was added. The nanostructures used were C nanospheres (NEC) and C nanoparticles (NPC), being the first one used only in the study of layer overlap (memories in stacked layers), since monolayer use has already shown success in a previous job [1]. The devices showed I_{ON}/I_{OFF} ratios of the order of 10^5 to 10^7, revealing efficiency through the great distinction of bit states "0" and "1 and minimum recording time with only 100ns.

[1] Hattenhauer I., Radomski F.A.D., Duarte C. A. and Mamo M. A., “Epoxy resin in organic WORM memories: from capsuling to the active layer”. Organic Electronics (2016) p. 57-66

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

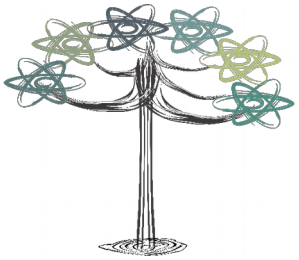
Study of Interaction of Small Molecules with Character of Internal Charge Transfer and Conjugated Polymers.

Anne Beatriz R. Abreu[1], Marlus Koehler[1] .

[1] *Universidade Federal do Paraná.*

In recent years the need to present new forms of energy generation has been intensified, motivating several studies in organic solar cells (OPVs). The literature on organic semiconductors extensive discusses the chemical-physical mechanisms that influence the efficiency of OPVs. One of those mechanisms is the charge transport that is particularly influenced by microscopic details related to the electronic coupling between molecules. In this work we investigated the intermolecular transfer integral t associated with a given electronic level. The transfer integral is related to the energetic splitting of this level when going from an isolated molecule to a system of interacting molecules. Turning to conjugated polymers, the splitting of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) level resulting from the interaction of adjacent chains along given directions yields the transfer integral that is used to describe the hole or electron transport in these directions. The computational method [1] used dimers in a particular direction, represented as fragments for the analysis coupling between molecular orbitals. The fragments investigated in dimers are constructed for different oligocenes and fluorenes molecules. Our preliminary results indicate that the integral transfer increases when silicon atoms replace carbon atoms in the molecules of the dimer. However, the transfer integral does not change when fluorine atoms replace carbon atoms in the molecules. Our approach can be generalized to calculate t for larger molecular complexes. We are especially interested to investigated the effect of the internal charge transfer (ICT) in oligomers of conjugated polymers in the transfer integral that coules those molecules.

[1] S. I. Gorelsky. AOMix: Program for Molecular Orbital Analysis; University of Ottawa, version 6.5 (2011). –www.sgchem.net/.



I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA

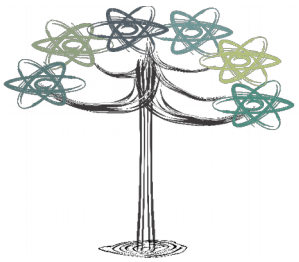
21 a 23 de Março de 2018

Semiclassical Dynamics of Entanglement for Longer Evolution Times

Arlans Juan Smokovicz de Lara, Alexandre Dias Ribeiro, Renato Moreira Angelo

Departamento de Física, Universidade Federal do Paraná

The study of entanglement generation in the semiclassical regime is an important issue in order to understand, for instance, to which extension it can be considered as a purely quantum concept, as commonly stated by the scientific community. In this work, we present a model of two particles, initially prepared in a product of coherent states, evolving in time according to a generic Hamiltonian, and derive a formula for the linear entropy of the reduced density matrix (an entanglement measure) for short times, using the semiclassical propagator in the coherent-state representation. The formula is exdplicitly written in terms of quantities that define the stability of classical trajectories of the underlying classical system, which somehow contradicts the standard belief. We will also present the tasks to be developed in the Master program, which essentially involve the improvement of the mentioned formula, extending its validity to longer times.



I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Vibrational population transference in a four level system using STIRAP and piecewise time-independent control methods

Aron L. O. dos Santos[1], Guilherme J. Delben[2], Marcos G. E. da Luz[3].

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[2] *Federal University of Santa Catarina – UFSC.*

[3] *Federal University of Parana - UFPR.*

Population transfer control has been extensively explored in the most diverse control methods. An effective procedure in the manipulation of physical properties in microscopic systems is an application of temporally delayed pulses, generating coherence and quantum superpositions. In the study of molecular processes, the stimulated Raman adiabatic passage – STIRAP - technique is efficient in the control of vibrational transitions in molecules composed of two atoms. Another method, considered new is the piecewise time-independent control - PTIC. Such a technique is based on solving inverse problems from an time-independent by parts approach. We aim to control a population transfer between the first four vibrational states of the OH molecule in the ladder configuration, aiming to populate the highest level. We use the Morse potential to model the diatomic molecule and solve a Schrödinger equation time-independent, thus determining the eigenfunctions and the energy eigenvalues. We applied the methods mentioned in the control of the OH radical and compared the profiles of the electric field of the laser, as well as the respective controlled populations. We verified that in the STIRAP technique three fields of radiation are used to control the target transitions, in contrast, in the PTIC method there are many different solutions to electric field, that can be implemented as a train of laser pulses inducing the population to the last vibrational level.

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Neuron dynamics variability and anomalous phase synchronization of neural networks

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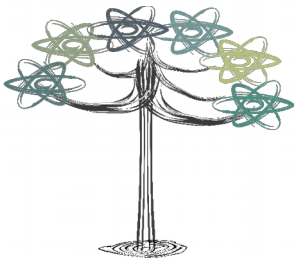
[1] *Departamento de Física – Universidade Federal do Paraná, Curitiba, Brasil.*

[2] *Instituto de Engenharia, Ciência e Tecnologia, Universidade Federal dos Vales do Jequitinhonha e Mucuri, Janaúba, Brasil.*

Anomalous phase synchronization describes a synchronization phenomena occurring for weakly coupled network and can be related to several neurological diseases, such as Parkinson and seizure behavior generated by epilepsy. Despite the success of control or suppress the anomalous phase synchronization in neural networks, applying external perturbations or inducing ambient changes, the origin of the anomalous phase synchronization, as well as the mechanisms behind the suppression are not completely known. Here, we consider a network composed of 2000 neurons with a small-world topology, and using two well known neuron models, namely a Hodgkin-Huxley like and a Hindmarsh-Rose models, both displaying anomalous phase synchronization. We show that the anomalous phase synchronization derives from the individual behavior of the neurons, particularly, we identify a strong correlation between the behavior of the inter-bursting-intervals of the neurons, what we call neuron variability, to the ability of the network to depict anomalous phase synchronization. We corroborate the ideas showing that external perturbations or ambient parameter changes that eliminate anomalous phase synchronization, also promote small changes in the individual dynamics of the neurons, such that an increasing individual variability of neurons implies in a decreasing of anomalous phase synchronization.



I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Distance correlation detecting Lyapunov instabilities, noise-induced escape times and mixing

Carlos F. O. Mendes, Marcus W. Beims

Universidade Federal do Paraná, 81531-980 Curitiba, PR, Brazil

The properties of the statistical method of distance correlation between multivariate data are analyzed in the context of nonlinear dynamical systems. The distance correlation between the noisy and the noiseless quadratic maps are studied in periodic and chaotic regimes. Results are compared to the classical method of Pearson's correlation. While distance and Pearson's correlations are affected by the Lyapunov exponent from the noiseless orbits, only the distance correlation is able to recognize the correct qualitative behaviour of escape times decays and the mixing of chaotic trajectories. The main goal of this work is to establish the validity of the distance correlation as an method of correlation between multivariate data in one-dimensional maps.

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Dynamic light scattering in a mixture of polyatomic gases: an alternative to obtain transport coefficients

Cesar Augusto Machado de Moraes[1], Wilson Marques Junior[1]

[1] *Universidade Federal do Paraná*

Different light scattering techniques have always provided important informations regarding the physical and chemical properties of materials. In fluids, or more specifically in gases, the study of the interactions between light and atoms provides informations about the dielectric constant and the transport coefficients. The characteristic scattering spectrum of gases in the hydrodynamic regime consists of three peaks and is called Rayleigh-Brillouin scattering. It is from the width, intensity and position of these peaks that the values of the transport coefficients can be estimated.

Lord Rayleigh,one of the first to study the blue-colored sky, wrote in his Scientific Papers that the origin of the light we are able to see is due to small suspended particles which divert from its regular course. As it is known from the classical theory of electromagnetism, the incident electromagnetic wave exerts a force on the particles, which accelerate and emit radiation. In order for a small volume of the fluid to emit scattered radiation, local fluctuations of the dielectric constant must be present. In this work, we considered that these fluctuations are functions of the usual macroscopic variables of thermodynamics: pressure, concentration and temperature of the mixture.

From the classical theory of electromagnetism it is possible to derive a relation between the scattered field and fluctuations in the dielectric constant. From the theory of correlation functions, it can be shown that the quantity called dynamic structure factor, which is measured in laboratories and is related to the intensity of the scattered light, is derived from correlations between the scattered electric field at different times, and, consequently, from dielectric constant deviations.

Therefore, the objective of this work is to calculate the dynamic structure factor for a binary mixture of polyatomic gases using a six field theory: density of the mixture, concentration of one gas, velocity of the mixture and temperature; and a nine-field theory, composed of one more equation for the diffusion flux. The hydrodynamic equations were obtained from the kinetic theory of gases.

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Outline of the "Grupo de Filmes e Nanoestruturas Magnéticas"

Dante Homero Mosca Junior.

Departamento de Física, Universidade Federal do Paraná

The research activities in magnetic films and nanostructures at UFPR started in 1994 with the support from the CNPq (certified: http://dgp.cnpq.br/dgp/espelhogrupo/8300347502831750). The research activities stretch over the disciplinary borders of physics and materials science. The present major researches are on the magneto-elastic behavior of ferromagnetic shape memory alloys (Ni-Mn-Ga and Ni-Mn-Ge) in thin films and rolled-up nanomembranes, spin currents in ferromagnetic films (Mn-Ga and Mn-Ge), nanomagnetism and biomedical applications of nanoparticles of transition metal nitrides (Cr-N, Fe-N, Ni-N, Co-N, among others) and non-conventional ferromagnetism in oxides (CeO_2, TiO_2, VO_x, among others). The research facilities concentrated in two laboratories (LSI and LANSEN) installed at Usina Piloto building contain instrumentation for the nanostructure fabrication by laser ablation synthesis in solution (LASiS) and molecular beam epitaxy (MBE) with *in situ* characterization by reflection high energy electron diffraction (RHEED) and photoelectron spectroscopies (XPS and UPS), as well as, a measure platform for magnetometry and magneto-transport (PPMS Evercool II, operational from 2 to 400 K @ 9 T). Current staff is formed by 3 professors, 1 senior-professor, 2 post-doc, 3 PhD students, 2 MSc students.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Study of photothermal effect in conjugated polymers nanoparticles

Marlus Koehler[1], Deize Corradi Grodniski[1]

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As one of the major causes of death, cancers or malignant tumors have greatly threatened human health. The development of new therapeutic agents or techniques with high specificity, low toxicity, and good patient compliance is of great importance for cancer treatment. In the past decade, photothermal therapy (PTT) that employs heat generated from the absorbed optical energy by light absorbing agents has attracted great attention. Inorganic nanoparticles have been used until now since they have strong optical absorbance in the near-infrared (NIR) tissue-transparency window. However, those inorganic nanomaterials that are not biodegradable could remain inside the body for long periods of time, raising serious concerns regarding their potential long-term toxicity.

The interest in thermal treatments was reactivated in the 1980s, after a while without news advances, when different institutes and societies focused on the understanding and development of novel thermal therapies were started. For the last few years, a great effort has been put not only into the development of novel techniques for controlled and localized heating but also into the understanding of the mechanisms at the basis of temperature induced cell killing and modification.

These thermal treatments consist in setting the temperature of a tumor within the 41-48 ºC temperature range (the so-called clinically relevant temperature range). Hyperthermia treatments are usually applied in combination with other cancer treatments, such as radiation therapy or chemotherapy, whose efficacy is increased when applied after a hyperthermia cycle.

However, NIR-absorbing conjugated polymer nanoparticles have been widely explored in biomedicine, by having excellent photostability, biodegradability, biocompatibility and high photothermal conversion efficiency. And recently, there has been a shift towards using conducting polymer nanoparticles based on polyaniline, polypyrrole and PEDOT:PSS, to photothermally treat cancer.

Heat generation in donor-acceptor conjugated polymers is not yet fully understood, however, it occurs through a slightly different process than carbon- and gold-based nanoparticles. It is hypothesized that, upon photoexcitation, an exciton is formed within the polymer. The exciton can then decay to a phonon band through lattice coupling with subsequent internal conversion generating heat.

In our work, P3HT poly(3-hexylthiophene-2,5-diyl) conjugated polymer nanoparticles were synthesized by nanoprecipitation method. A green laser beam (532 nm) operating at 30mW was used to photoexcitation.

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Electronic Structure and Optical Properties of $LaNiO_3$

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Among various transition metal oxides, LaNiO3 arouses great interest on its physical properties, such as strong electron-electron correlation and metal-insulating transition (MIT). This compound is from the perovskite family and has paramagnetic metallic character, with strong electronic correlation between Ni 3d and O 2p orbitals. It has a rhombohedral structure with pseudocobic lattice (R3c spacial group). Its lattice is interconnected by octahedros NiO6 with binding angles Ni-O-Ni slightly distorted when compared with ideal perovskite crystalline structure.The presented results were calculated by Density Funtional Theory (DFT) using the Wien2k computational package. The approximation used for the exchange-correlation potential was generalized gradient approximation (GGA). The obtained results for density of states and dieletric function were calculated near to the Fermi level, where shows the strong correlation effects. These results were compared with measures of photoemission, absorption and dieletric function reported in the literature. In comparison, the calculations are in agreement with the experimental results. The good agreement between calculated and experimental results shows the efficiency of the method used, which can be implemented for studies of similar structures.

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Jeans Instability for a System of Two Components in an Expanding Universe

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The present work seeks to analyze the dynamics of a self-gravitating fluid composed by baryonic and dark matter within the framework of the Poisson equation and the collisionless Boltzmann equation in an expanding universe. The Jeans instability is connected with the density contrasts, which indicate the local increase of baryonic and dark matter densities. It is shown that the dispersion velocities ratio between dark matter and baryonic matter has influenced on the Jeans masses. For larger wavelengths, the density contrasts grow with time while for small wavelengths they have an oscillatory behavior.

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Photovoltaic Devices based on Metal Oxide Heterostructures

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The searching for new alternative sources of sustainable energy, has been intensified in recent years due to the need to minimize the environmental impacts caused by conventional sources of energy. In this context, the solar energy is an attractive alternative, although it is still necessary to overcome many obstacles. Basically the conversion of solar energy into electrical energy takes place through a structured photovoltaic device in the sandwich-shape. Essentially, the light enters the active layer of the device by the transparent electrode promoting the generation of electron-hole pairs in the active layer in the vicinity of that electrode. The formed pair needs to diffuse to a dissociation interface, without recombination, and after the pair has been dissociated, the holes follow to the hole collecting electrode and the electrons are transported to the electron collecting electrode generating a photocurrent. There are several factors that limit the efficiency of these devices, one of which is the low long term stability. The manufacture of photovoltaic devices composed of layers of metal oxides has become quite attractive due to its greater stability, considering that the metal oxides are highly stable. Therefore, this work focus on the manufacture and characterization of photovoltaic devices composed of heterostructures of metallic oxides, consisting of an active cuprous oxide layer (Cu_2O). This layer was chosen especially for its excellent optical and electrical properties, although Cu_2O does not have an ideal optical gap (~ 1.4 eV) for solar energy conversion. According to the Shockley-Queisser limit, Cu_2O with a band gap of 2.17 eV is an efficient active layer for the absorption of sunlight when compared to other metallic oxides. A layer of nickel oxide (NiO) will serve as a collector of holes and layer of zinc oxide (ZnO) as an electron collector. A transparent electrode (ITO – Indium Tin Oxide) and an evaporated aluminum electrode (Al) complete the device. This work was divided into two parts, the first being focused on the separate synthesis, preparation and characterization of the thin films of metal oxides and the second on the photovoltaic device manufacture and characterization. The results presented here will be related to the first part of this work with the structural, morphological, optical and electrical characterization of thin films of metallic oxides.

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Modelling of transport phenomena *ab initio*

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All kinds of calculation of gas flows use some potential of intermolecular interaction. The widely used phenomenological potentials such as hard spheres, Lennard-Jones, Stochmayer, variable hard spheres, variable sort spheres, contain several fitting parameters usually extracted from experimental data on transport coefficients (viscosity, thermal conductivity, diffusion) or from virial coefficients. Recently, the potentials for many gases and their mixtures have been calculated from main physical principals applying quantum-mechanical calculations. The group “Rarefied gas dynamics” at Physics Department of UFPR implemented these potentials to solve the Boltzmann equation, see e.g. the works [1,2], and to apply the direct simulation Monte Carlo method, see e.g. papers [3-5]. These results showed that some phenomena like mass flow rate, shear stress and heat flux in a single gas with a small temperature variation are not sensitive to the potential so that the simplest potential like the hard sphere model can be successfully used if the molecular diameter is well adjusted. However, some phenomena in gaseous mixtures like diffusion and thermodiffusion are strongly sensitive to the potential and should be modeled applying *ab initio* potentials when available. In the presentation, recent results on gas flows based on *ab initio* potentials will be reviewed. A comparison of results based on *ab initio* with those obtained using phenomenological potentials will be performed.

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Structure of planar shock waves in gaseous mixtures. Ab initio direct simulation.

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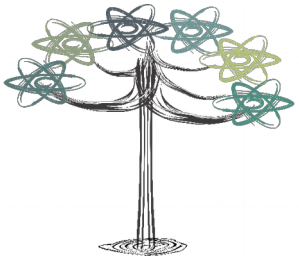
The structure of planar shock wave propagating through a helium-argon mixture is modelled by the direct simulation Monte Carlo (DSMC) method based on ab initio potentials for a wide range of the Mach number and for various molar fractions. The use of the ab initio potentials allows us to carry out the simulation without any adjustable parameter usually extracted from experimental data. As a result, the density, temperature, molar fraction, diffusion velocity, pressure tensor and heat flow profiles inside of the shock wave are calculated and the temperature overshoot phenomenon is studied in details. The slopes of density are calculated with the numerical error less than 0.5 %. It is pointed out that the slopes for mixture are always smaller than those for a single gas.



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Critical noise amplitude in Chua's circuit model

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The canonical Chua's circuit model is described by three coupled first-order autonomous differential equations and presents a rich variety of dynamics as a function of the parameters, i. e., the voltages across the two capacitors,and the current across the inductor. Usually, the nonlinear model for Chua's diode uses a piece-wise linear curve for its current-voltage characteristic. Recently, it was reported some experimental results in the inductorless version of the Chua circuit, showing deformations in its parameter space. Besides, it is well known that noise and temperature may cause fluctuations in the values of the electronic components, for example, in the resistors and in the operational amplifiers. Some works report that these fluctuations change the parameter spaces of dynamical systems. In this work, we study the effect of noise in the inductorless Chua's circuit model by solving numerically the equations of the circuit using a fourth-order stochastic Runge-Kutta integrator. As a model, we use a gaussian noise which is added to one of the equations. The main goal is to find the critical noise intensity which transforms the regular periodic motion in a chaotic one. Results are presented in the parameter space. With this model we expect to describe instabilities found in the corresponding experimental results.

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Characterizing the transient dynamics towards stationary Lévy reaction-diffusion processes

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In random search model the search environment play a important role. In these models, several realization of the same search parameters are performed with different randomly generated landscape, to obtain the sufficient number of avarages for the statistical analysis. The total number of the targets remain constant, although its distribution in the space changes at every new simulation. In this work we present an analitycal and numerical model to describe transient dynamics towards stationary in Lévy processes. The density of resources on the search evironment increases over time until the limit stationary is reached. We characterize the bahavior of the dynamic search enviroment by means of two processes: targets creation and targets annihilation. Every time the searcher covers a characteristic length τ , the environment will recieve one new target at a random position. For searches strategies $\mu = 1.0$. our model have exact solution and the result match with numerical simulation very well. We characterizes by means of analitycal function, the physical quantities like availabel targets, detected targets and search efficiency e we shown that behavior of this quantities during transient times is like exponencial.

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Positron Scattering by Formic Acid Complexes

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One reason that makes the study of the interaction of positrons with biomolecules interesting is the positron emission tomography (PET) technique. Studies by Robson *et al.* [R. E. Robson, M. J. Brunger, S. J. Buckman, G. García, Z. Lj. Petrovic, and R. D. White, *Sci. Rep*. **5** , (2015)] show the need to more accurately treat the structure of the medium in PET simulations, that is, as more than 60% of the human body is made up of water, it is important to know how positrons behave in this environment. Therefore, our interest is to study the scattering of positrons by microsolvated systems. Based on the motivation presented, we chose for this study the formic acid molecule, since this plays an important role in the formation of large molecules, such as glycine and acetic acid. The microsolvation's influence in the formic acid the has been studied in the electron scattering [T. C. Freitas, K, Coutinho, M. T. do N. Varella, M. A. P. Lima, S. Canuto, and M. H. F. Bettega, *J. Chem. Phys.* **138** (2013)]. In this work, we report the integral cross sections for elastic collisions of low energy positrons with the $HCOOH\cdots H_2O$ complexes. In the scattering calculations we employed the Schwinger Multichannel Method (SMC) [J. S. E. Germano and M. A. P. Lima, *Phys. Rev. A* **47** (1993)] in the static plus polarization (SP) approximation for energies ranging from 0.5 eV to 10 eV. We also include the contribution of the permanent electric dipole moment of the complexes through the Born-closure approximation. Formic acid has two stable isomers, namely cis and trans. In the calculations, we considered ten different structures hydrogen-bonded structures of $HCOOH\cdots H_2O$ (being five isomers cis and others five trans) which were generated using classical Monte Carlo simulations [K. Coutinho and S. Canuto, *J. Chem. Phys.* **113** (2000)] of acid formic in water environment at room temperature. We also carried out calculation for the HCOOH (cis and trans) in gas phase for purpose of comparison with the complexes results.

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Nitride nanoparticles synthesized by laser irradiation in liquid nitrogen

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The magnetic properties of nanocrystalline materials can differ significantly from the corresponding bulk material. Particularly, magnetic nanoparticles (NPs) offer various advantages for applications as magnetic fluids, catalysis, or magnetic energy storage. Besides, the use of magnetic nanoparticles is arising in fields of biology and medicine with methods like cell-sorting, hyperthermia, or magnet resonance tomography [1]. Magnetic NPs are very well suited to these purposes, as their size makes them easy to be embedded within a variety of materials where they can be exposed to static and/or alternating magnetic fields [2]. This work focuses on NPs of transition metal (Fe, Co, and Ni) nitrides synthesized by laser ablation in liquid nitrogen. Indeed, the nanomaterials are obtained by irradiation of laser pulses on a bulk target immersed in liquid nitrogen. We used to synthesize NPs a Nd: YAG (neodymium-doped yttrium aluminum garnet) Quantel (model Brilliant B) laser. The resulting NPs were collected after nitrogen evaporation and used to prepare suspensions in water, isopropyl alcohol, and saline solution. Their size distribution and shape were analyzed by transmission electron microscopy (TEM), whereas selected area electron diffraction (SAED) were used to identify the nanomaterial phases and structures. Moreover, magnetic measurements using a vibrating sample magnetometer (PPMS Evercool II) were performed.

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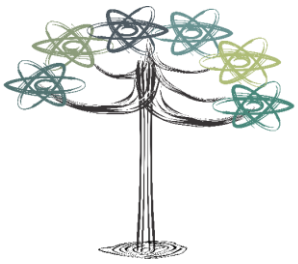

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The Emergence of Large Polarons in $CH_3NH_3PbI_3$ Perovskite

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The electron-phonon coupling due to an excess charge in organic halide perovskites may be strong enough to result in a self-trapped polaron. These polarons have effective sizes much larger than the bond-length and travel through a lattice as free electrons but with an enhanced effective mass, which can explain the observed low electron-hole recombination rates and modest mobility in organic halide perovskites. Using Monte Carlo and electronic structure calculations we investigate the emergence of large polarons in $CH_3NH_3PbI_3$ perovskite.

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Organic Transistors Based on Poly(3-hexylthiophene-2,5-diyl): Latest Achievements and Major Constraints Requiring Research Efforts

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In the last years our group has investigated field-effect transistors based on poly(3-hexylthiophene-2,5-diyl) (P3HT) semiconductor and poly(vinyl alcohol) as insulator, aiming device performance melioration [1-8]. In this contribution, the strategies developed so far to improve key transistor performance-determining parameters will be discussed, also presenting main factors that hinder further improvements and require additional research efforts. The consequences of the use of defect-free, 100% regioregular, P3HT [6] on positive charge carrier field-effect mobility will be shown, comparing the results with those obtained with lower regioregularity P3HT. The influence of the regioregularity of P3HT on the molecular interaction of P3HT molecules with polar functional groups of the FET insulator surface [2,4-5] will also be addressed, since it strongly affects the molecular order and the charge transport properties of organic FETs. The newest achievement of field-effect mobility of 6 $cm^2/V.s$ by using P3HT molecules aligned to the charge flow direction in the transistor channel will be presented [8]. Finally, the main constraint hindering the preparation of high field-effect mobility and high source-drain current transistors will be discussed, proposing strategies to overcome present bottlenecks.

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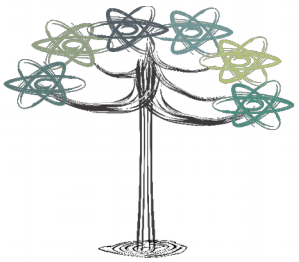

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Rydberg molecular systems: From antiprotonic Helium to Trilobites in a dense gas

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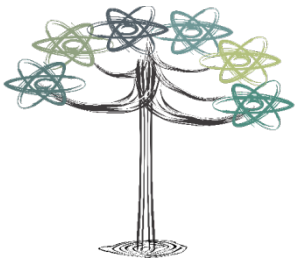
Highly excited "Rydberg" systems play an important role for progress in theory, experiment, and more recently for potential applications in quantum computing. Rydberg systems connect ultracold physics, condensed and atomic/molecular physics and also non-linear (semi-)classical dynamics on the theoretical side. In the talk I will illustrate this progress with exotic Rydberg systems from antiprotonic helium to ultralong-range Rydberg molecules with several thousand atomic units bond length. Immersed in their natural environment of an ultracold gas those molecules thrive through the presence of many randomly located gas atoms – a surprising and counterintuitive result. It is rooted in a novel scarring phenomenon of excited quantum wave functions and the fact that a random gas contains clusters of atoms, a phenomenon more broadly known as "birthday paradoxon".



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Self – Gravitating systems of ideal gases in 1PN approximation

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We obtain the Maxwell-Jüttner distribution function at 1PN approximation within the framework of general relativity. Taking into account the aforesaid distribution function, we compute the particle four-flow and energy-momentum tensor. We focus on the search of static solutions for the gravitational potentials with spherical symmetry. In doing so, we obtain the density, pressure and gravitational potential energy profiles in terms of dimensionless radial coordinate by solving the aforesaid equations numerically. In particular, we find the parametric profile for the equation of state p / ρ in terms of the dimensionless radial coordinate. Due to its physical relevance, we also find the galaxy rotation curves using the post-Newtonian approximation. We join two different kinds of static solutions in order to account for the linear regime near the center and the typical flatten behavior at large radii as well. Finally we compared our rotation curves with observational data of spiral galaxies.

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Molecular dynamics of conjugated polymer systems*

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The growing demand for new forms for generation of renewable energy has motivated many researchers during the last years. In this field, organic photovoltaic devices (OPVs) based on donor/acceptor heterojunctions, have promoted great interest in the scientific community due to the unique properties of organic materials, such as lightness, easy manufacture, high flexibility and low cost **[1]**. Solar cells containing polymers, as electron donors and fullerene derivatives as electron acceptors, achieved energy conversion efficiency between 8.7% and 11.5% **[2]**. Different solvents influence many electrical and optical properties, such as, polymer backbone conformation, solubility, absorption, charge carrier mobility and energy levels. It is possible to control the system morphology with the addition of co-solvents (additives) in the main solvents. This process modifies the polymer planarity and increases the OPV device efficiency. However, it is not well understood the physico-chemical processes involved in those changes, especially in variations of the polymer. In this work, we study by computational simulation the polymer poly[(9,9-dioctylfluorenyl-2,7-diyl)-bithiophene] (F8T2) solubilized in the solvent chlorobenzene (CB), with/without 1,8-diiodooctane (DIO) additive. Our focus is to study the physical phenomena related to the morphology of the resulting thin film. Thus, we use molecular dynamics by appliyng the GROMACS package **[3]** to simulate the F8T2/CB:DIO system. In addition, we perform quantum chemistry calculations to optimize the parameters of both, the functional groups within the polymer, and the solvent molecules. We present some techniques for parameterization and simulated evaporation **[4],** in order to correlate with experimental results. Our preliminary results shown sufficient correlations between our model and experiments.

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Theoretical study of the effects of solvent additive on conjugated copolymer based on fluorene and bithiophene

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[3] *University of California Berkeley*

In the last years the use of solvent additives for fabrication of polymeric thin films has become an important procedure to induce morphological changes at the system nanoscale [1,2]. Yet the effects of those additives on the polymer's backbone conformations (with variations on the electronic structure) remains elusive. By combining our theoretical chemistry simulations with experimental results [3], we show that the use of the solvent additive 1,8-diiodooctane (DIO) can alter the conformation of poly[(9,9-dioctylfluorenyl-2,7 diyl)-co-bithiophene] (F8T2) chains resulting in improved properties of the film. We have simulated F8T2 oligomers with five repeated units with two different conformations: one with the S atoms of the thiophene ring pointing to the same direction, named syn conformation, and another with the S atoms pointing to the opposite direction, called anti conformation. The results suggests that the solvent additive induces a higher density of syn conformers in the bithiophene unit of the copolymer backbone, planarizing the polymer's geometry. The simulations indicate that this transition is possibly mediate by the interaction between the iodine atom of the DIO and the heteroatoms of the bithiophene moiety. The higher degree of electronic delocalization and the enhancement of the interchain interactions improves the transport and the photovoltaic features of F8T2 layers. The application of solvent additive treatment to provide conformational changes of the backbone can be a favorable strategy to improve optoelectronic properties of polymer-based devices.

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Temperature oscillations in circular geodesic motion of a gas in Reissner-Nordström field

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The objective of this work is to analyze the temperature oscillations that occur in a gas in a circular geodesic motion under the action of a Reissner-Nordström gravitational field, verifying the effect of the charge term of the metric on temperature oscillations. The expression for the temperature oscillations follows from Tolman's law written in Fermi normal coordinates for a comoving observer. From this expression, the oscillations are calculated for some compact stars, quark stars, black holes and white dwarfs, using values of electric charge and mass from models obtained in the literature. Comparing the various models analyzed, it is possible to verify that the role of the charge is the opposite of the mass. While the increase of the mass produces an increase in the frequency and a reduction in the amplitude and in the ratio between the frequencies, the increase of the electric charge produces an inverse effect. In addition, it is shown that if the electric charge is proportional to the mass, the ratio between the frequencies does not depend on the mass, but only on the proportionality factor between charge and mass. The ratios between the frequencies for all the models analyzed (except for supermassive black holes) are close to the 3/2 ratio for twin peak quasi-periodic oscillation frequencies observed in many galactic black holes and neutron star sources in low-mass X-ray binaries.

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21 a 23 de Março de 2018

Electron collision with cyanamide: shape resonances and dissociation

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Cyanamide (NH_2CN) is a multifunctional compound widely used in agriculture such as pesticide and plant growth inhibitor. As opposed to what was known, it is a natural product formed in some plants. In addition, the cyanamide is one of the rare interstellar molecules that contain two atoms of nitrogen and is recognized as an important prebiotic molecule, a key point to understanding the origin of life.

There are few studies regarding electron interactions with cyanamide molecule. One of these studies have reported dissociation cross sections (Tanzer *et al.* [J. Chem. Phys. 142, 034301, 2015]) and the other one have presented the integral elastic and electronically inelastic cross sections for low-energy electrons scattering by NH_2CN obtained with R-matrix method (Wang *et al.* [Phys. Rev. A 94, 032703, 2016]). About the last one, the authors identified two resonances (one π^* and one σ^*) in their elastic cross sections and proposed that the low lying π^* resonance is linked to an indirect dissociation when the $C-N$ single bond is elongated.

Then, the main goal of this work is to investigate the existence of this indirect dissociative electron attachment (DEA). We performed electronic structure calculations to obtain the energy of the unoccupied orbitals associated via Koopmans' theorem to the π^* and σ^* resonances. Using these energies, we also construct the potential energy curve for the neutral cyanamide and for the anion states as function of the $C-N$ bond stretching. As a result, we show that the curves of the π^* and σ^* anion states cross. So there is an exchange between the π^* and σ^* resonances while maintaining the initial symmetries.

Finally, we also present the elastic cross sections for low-energy electron collisions by cyanamide. Our calculations employed the Schwinger multichannel method (SMC) implemented with pseudopotentials and were performed in the static-exchange (SE) and static-exchange plus polarization (SEP) approximations. We identify two shape resonances which are positioned in energies near of the energies reported for Wang *et al.*. The scattering calculations were also performed for the stretched geometries.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Thin films of conducting polymers, Carbon Nanotubes and Graphene oxide: their use in electronic devices in the group of Nanostructured Devices (DiNE)

Lucimara Stolz Roman

Universidade Federal do Paraná.

Research efforts on thin film mixtures of conducting polymers and carbon nanostrucutures have created new possibilities for electronic devices. Several materials and, combinations of materials, have been presented in many device configurations along the last years. Here, we present our studies on optical, morphological and electrical properties of thin nanostructured films active layers used for different purposes, such as, electrodes of Organic Photovoltaics (OPVs), active layers for OPVs and active layers in gas sensors. The films are obtained by (i) simple mixture in a common solvent, (ii) miniemulsion technique or (iii) generated by interfacial synthesis. (i) Using simple mixture between graphene oxide (GO) and PEDOT:PSS with different content ratios was possible to achieve an environmentally friendly, conductive, transparent and flexible thin film in which the composite features are betters than the compounds separately used as transparent electrodes in organic solar cells . (ii) The miniemulsion technique allows the nanostructuring of polymers in aqueous solution and offers significant potential advantages and we present an easy method to synthesize polymer nanoparticles using graphene oxide as an alternative to the traditional insulating surfactants, using the Pickering emulsions concept. (iii) The interfacial polymerization method to synthesize carbon nanotubes/polyaniline composites, in which the final material is obtained as a thin film at the liquid-liquid (water/oil) interface; according the ratio between polyaniline and carbon nanotubes, the film morphology is represented by a continuum of polymer containing CNTs embedded in it, or by touched CNTs individually capped by a thin polymer shell. Here is presented the electrical characteristics of these films as well as their use as transparent electrodes in ITO-free organic photovoltaic devices and gas sensors.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Studies on the influence of post annealing treatment and additives on bulk heterojunction OPVs

Maiara de Jesus Bassi[1], Luana C. Wouk[1], Camilla C.K. Oliveira, Lucimara Stolz Roman[1]

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The structure of organic solar cells based on bulk heterojunction, in which an electron donor and acceptor materials are blended, increases the interfacial area between these materials and enables the active layer deposition in only one step. The mixing between conjugated polymers and fullerene derivatives still is the most widely used active layer in OPVs. The ordering, crystallinity and interpenetration in organic materials are modified by thermal treatment and solvent evaporation rate. Thus, the reorganization energy and different deposition techniques could affect the devices performance. In this work we studied how the post annealing temperature and additive 1,8-Diiodoactane (DIO) influences on devices efficiency. A blend using poly[2,7-(9,9-dioctyl-dibenzosilole)-alt-4,7-bis(thiophen-2-yl)benzo-2,1,3-thiadiazole] (PSiF-DBT) as donor materials and [6,6]-phenyl C_{71} butyric acid methyl ester ($PC_{71}BM$) as electron acceptor. For these systems, there was not a significant improvement with annealing at 100 ° C and, at 200 ° C the active layer was bleached. The improvement came with the use of DIO in the active layer. Optical, morphological and electrical measurements for these attempts will be presented and discussed.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Vertical Architecture Organic Thermoelectric Devices

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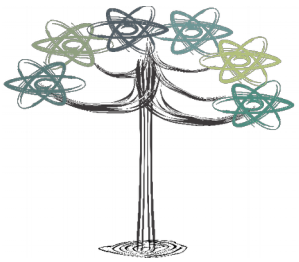
In this work, vertical architecture organic thermoelectric devices based on the Seebeck Effect are prepared and studied. Thermoelectric devices are an emergent alternative to obtain energy from wasted heat sources. Organic thermoelectric devices show lower efficiency than the inorganic ones but exhibit some advantages like easy processability, low costs and flexibility, which make them an interesting and prominent alternative to be studied. The devices presented in this work are prepared in the laboratory of the Group of Organic Optoelectronic Devices at Universidade Federal do Paraná (UFPR), where every layer of each device is assembled by a specific process of synthesis. They consist basically of bottom ITO (indium tin oxide) contact layer, which is adhered to the substrate, a polymer thin film (active area) of SPAN (sulfonated polyaniline) deposited over the bottom contact and a top Al contact evaporated over the SPAN film. The process to make these devices can be summarized by the following steps: ITO is partially etched and, in the sequence, it is submitted to cleaning process followed by UV-Ozone treatment. The thin films are prepared through chemical deposition, where the ITO is placed face-down on the surface of the precursor solution. In this way the thin film is deposited on the ITO surface. In the last step Al electrode is evaporated under base pressure of 5×10^{-6} torr. The structure of the thermoelectric device is vertical along with the measurement. This facilitates charge transport in the polymer film due to the short path, which is approximately the thickness of the film, in contrast to horizontal structures where the path is usually much larger. The Seebeck coefficient of the device is estimated by the ratio of the curves of the induced voltage difference and the difference of temperature of the device. The temperature difference is obtained by using two thermocouples through the measurement of a local voltage, which is converted to temperature. The induced voltage due to thermoelectric effect is measured by two probes. Thickness of the thin film is obtained with a profilometer.



I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Collisions of low-energy electrons/positrons with molecules

Márcio Henrique Franco Bettega, Sergio d'Almeida Sanchez

Departamento de Física, Universidade Federal do Paraná

We are a "subgroup" of the Atomic and Molecular Physics (AMoP) group. The AmoP also includes Prof. Milton Massumi Fujimoto, who works in electron collisions with molecules and uses several different methodologies to treat this problem. AMoP also includes Profs. Marcos Gomes Eleutério da Luiz and Marcus Werner Beims, who study caos in atomic and molecular physics. Prof. José Arruda de Oliveira Freire is also member of the AMoP group and works with electronic transport in organic molecules.

There is a list of topics that motivate theoretical and experimental studies of low-energy electron and positron collisions with molecular targets, e.g., modeling of "cold" plasmas for chemical vapor deposition and etching, molecular fragmentation induced by electron attachment (a process that occurs in DNA and motivated studies on biological molecules) and diagnosis of tumors using positron emission tomography. In electron collisions with molecules, the main focus of our studies has been the shape resonance spectra. Resonances can mediate molecular dissociation, and the knowledge of their nature, energy and width is important in the understanding of the dissociation process. These resonances are identified by looking at the scattering cross sections. Electronic structure calculations also help in the characterization of the shape resonances. Scattering of positrons by molecules is a challenge for the theorists, since the positronium (Ps) formation channel has a large contribution for the total cross section when this channel is open. Our group has focused in the description of the collision process below the positronium formation channel. In this workshop we will present some recent results obtained by our group for electrons/positrons collisions with molecular targets. The cross sections are computed using the Schwinger multichannel (SMC) method, which is a variational method for the scattering amplitude. For electron collisions the exchange and polarization interactions are included in an *ab initio* fashion; in positron collisions (no exchange), polarization effects are also described *ab initio*.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Ratchet systems and extreme events

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This talk presents an overview of our recent results about the description of nonlinear dynamical systems. More specifically, we describe the optimization of the ratchet transport along periodic structures and the prediction of extreme and rare events in chaotic three-dimensional systems.

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21 a 23 de Março de 2018

Quantum thermodynamics of simple systems

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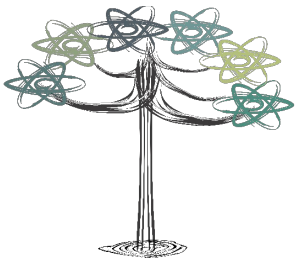
Definitions of physical concepts, such as work and heat, are well established in standard thermodynamics. However, when applied to systems far below the macroscopic limit, in which size effects, quantum phenomena, and non-equilibrium regimes are ordinary, these quantities need to be reformulated. Quantum thermodynamics is the emergent research area where this discussion takes place. In this work, we present this subject, revisiting some models of heat machines and simple quantum systems, in order to introduce a panorama of this new approach and identify interesting questions to be studied.



I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
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Electron scattering from C4H6, C5H8 and C6H10 molecules

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In this work we report calculated elastic differential and integral cross sections for electron collisions with 1,3-butadiene (C4H6), 2-methyl-1,3-butadiene (C5H8) and 2,3-dimethyl-1,3-butadiene (C6H10) molecules, for impact energies up to 20 eV. We investigated the methylation effect (the substitution of a hydrogen atom by methyl group) in the shape and magnitude of the cross sections. The present results are compared with the experimental total cross sections available in the literature. Our calculations were performed with Schwinger Multichannel Method with pseudopotentials in the static-exchange and static-exchange-polarization approximations. For the polar molecule 2-methyl-1,3-butadiene, we included the Born closure procedure in order to account for the long-range potential. We found two shape resonances (formation of negative ion states when the incoming electron is temporarily captured into an unoccupied molecular orbital) bellow 4.5 eV for each one of the three molecules studied. We also discuss the differences between our results and the experimental data. We showed that the Ramsawer-Townsend minimum ,observed around 1.6 eV in experimental data for C5H8, is actually a valley between the two shape resonances. Also for C5H8 molecule, the enhancement bellow 1.6 eV reported by the experiment is due to the presence of a low-lying shape resonance and not an effect due to its permanent dipole moment. In general our results are in good agreement with the experimental data.

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21 a 23 de Março de 2018

Electronic structure of transition metal oxides

Miguel Abbate[1]

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The electronic structure of transition metal oxides is strongly influenced by electron correlation effects. These effects result in materials with a broad range of very interesting physical properties. For instance, high-T_C superconductivity, colossal magneto-resistance, metal-insulator transitions, etc. In our group, we study the electronic structure of these compounds using experimental and theoretical techniques. The main experimental techniques are X-ray photoemission and X-ray absorption spectroscopy. The theoretical methods include band structure calculations, as well as exact diagonalization of Hubbard models. The main goal is to relate the electronic structure to the microscopic origin of the physical properties. We will present our main contributions in this area, as well as the main results of the students of our group.

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Electron Scattering by Molecules of HOOCl

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In 1974, Rowland and Molina found that chlorine atoms produced by the UV irradiation of chlorofluorocarbons (CFCs) are involved in the ozone depletion. Since then, several models of reactions have been proposed for ozone depletion, where HOOCl plays an important role as a reaction intermediate. However, there is no experimental data about this molecule, because it is very unstable molecule and it has never been identified experimentally. Therefore, the objective of this work is to perform a study of the interaction of low-energy electrons (1-10eV) and molecules of HOOCl in the gas-phase. The target description is performed by Hartree-Fock method in the fixed-nuclei approximation. In this work, the interactions between free electrons and HOOCl molecules were studied and differential and integral cross sections were calculated using the UK-Matrix-R method. In the R-Matrix formulation the space is split into an inner and an outer region limited by a sphere of radius which is a multiple of the Bohr radius, centered on the center of mass of the molecule. In the inner region short range effects such as polarization, exchange and correlation effects are taken into account. And in the outer region long range effects, like the interaction of the free electron with the dipole are considered. In this work, several kind of tests were performed, such as: 1) comparison between different atomic basis for the molecule description; 2) radius variation of the sphere which divides the inner and outer regions; 3) inclusion or not of the polarization effect of the electronic cloud of the molecule; 4) inclusion or not of the Born-closure correction for the analysis of the long-range effects. The tests were performed to observe what are their effects on the cross section and to ensure that a reliable cross section will be obtained. During the workshop we will present how each one of the factors affect the results, as well as, the final cross section which we consider more reliable.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Magnetic coupling in CeO_2/[Co/Pt]$_5$ multilayered heterostructures.

FIGUEIREDO-PRESTES, Nicholas[1], ZARPELLON, Juliana[1], JURCA, Hugo F.[2], FERNANDES Vilmar[3], VARALDA, José[1], SCHREINER, Wido H.[1], MOSCA, Dante H.[1], FICHTNER, Paulo F. P.[4], FABRIM, Zacarias E.[4], BOUZEHOUANE, Karim[5], DERANLOT, Cyrile[5], GEORGE Jean-Marie[5].

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[5] Unité Mixte de Physique, CNRS, Thales, Univ. Paris-Sud, Université Paris-Saclay;

Materials with perpendicular magnetic anisotropy (PMA) are of great interest as they have potential applications in high-density non-volatile memories, spin logic devices, and other spintronics applications. To attain perpendicular anisotropy, several material systems have been explored as ferromagnetic electrodes. Here, we use (Co/Pt)-multilayered films with PMA covered by a gold spacer-layer to induce the perpendicular magnetization in a ferromagnetic layer of cerium oxide and to control the reversible switching of its magnetization. The origin of the room-temperature ferromagnetism observed in nanocrystalline cerium oxide films remains controversial, but their wide energy band-gap and their transparency to visible light attracts attention for possible applications in magneto-optical devices. A weak magnetic stray field of 40 Oe emanates from the (Co/Pt)-multilayered film and permeates the gold spacer layer. Using a simple micromagnetic model based on the Stoner–Wohlfarth magnetization mechanism, the strength of the magnetic coupling between the ferromagnetic layers is estimated to be 18 uJ/m2. This magnetic coupling, which is almost independent of temperature, is sufficient to promote the reversible switching of perpendicular magnetization states in the field range of only a few hundred Oersteds at room temperature.

This work has been published by RSC Advances. More information at https://doi.org/10.1039/C6RA10392H

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Information-reality complementarity: The role of measurements and quantum reference frames

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Recently, a measure has been put forward which allows for the quantification of the degree of reality of an observable for a given preparation [A. L. O. Bilobran and R. M. Angelo, Europhys. Lett. **112**, 40005 (2015)]. Here we employ this quantifier to establish, on formal grounds, relations among the concepts of measurement, information, and physical reality. After introducing mathematical objects that unify weak and projective measurements, we study scenarios showing that an arbitrary-intensity unrevealed measurement of a given observable generally leads to an increase of its reality and also of its incompatible observables. We derive a complementarity relation connecting an amount of information associated with the apparatus with the degree of irreality of the monitored observable. Specifically for pure states, we show that the entanglement with the apparatus precisely determines the amount by which the reality of the monitored observable increases. We also point out some mechanisms whereby the irreality of an observable can be generated. Finally, using the aforementioned tools, we construct a consistent picture to address the measurement problem.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Steering multiattractors to overcome parameter inaccuracy and noise effects

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Steering of attractors in multistable systems is used to increase the available parameter domains which lead to stable dynamics in nonlinear physical systems, reducing substantially undesirable effects of parametric inaccuracy and noise. For discrete nonlinear systems, the purpose is to apply a recently proposed methodology [1,2] to enlarge parameter domains for which optimal ratchet currents (RCs) are obtained. This task is performed by adding a suitable periodic perturbation F_j on a Ratchet mapping and the procedure consists in multiplying a specific class of Isoperiodic Stable Structures (ISSs), since the existence of nonzero RCs is directly related to the occurrence of stable domains. By proliferating the ISSs, it is possible to: (i) postpone thermal effects that usually increase the chaotic domain and (ii) demonstrate, by using a quantitative analysis, that the area which provides optimal RCs in the two-dimensional parameter space can be enlarged around 78%. In addition, for some specific parameter combinations, nonzero RCs can be induced through the birth of a new attractor, which moves away as the strength of F_j increases. For continuous systems, the procedure proposed here uses suitable perturbations to move independent multistable attractors in phase space. By applying this mechanism, we increase roughly 85% the ratchet current described by the Langevin equation and 60% the Lyapunov stable domains in Chua's electronic circuit. Our proposal is expected to have wide applications in generic nonlinear complex systems presenting multistability, so that related experiments can increase robustness under parametric inaccuracy and noise.

[1] R. M. da Silva, C. Manchein and M. W. Beims. Chaos **27**, 103101 (2017).

[2] C. Manchein, R. M. da Silva and M. W. Beims, Chaos **27**, 081101 (2017).

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Coupling among nonlinear oscillators mediated by a diffusing substance

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In this work, a general theory is presented for the coupling among nonlinear oscilattors mediated by a diffusing chemical substance. We extend a model developed by Kuramoto, who supposed that the diffusion characteristc time is much shorter than the oscilltor main period, such that diffusion occurs very fast. But this model fails if the diffusion time is comparable or is much bigger than the oscillator period. To work this case, we eliminate this constraint and consider diffusion to have an arbitrary characteristic time, by solving exactly the diffusion equation using suitable Green functions. We present results for the Green functions in one, two and three dimension, in the free space.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
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Synthesis and characterization of Se_9Sn semiconductor alloy

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This work presents a study developed in the Laboratory of Synthesis and Characterization of Materials (LSCM), oriented by Prof. Dr. Kleber Daum Machado, regarding the production and characterization of the amorphous chalcogenide alloy Se_9Sn. The interest in chalcogenide glasses is due to its great technological potential applied to many applications, such as optical devices, optical sensors that perform some function when interacting with light, optoelectronic, solar cells or CCD cells, electronic, thermoelectric devices, among other applications. About Se_9Sn alloy, we are proposing a more detailed study about the atomic structure of this amorphous alloy, which is very important, because recent research gives more emphasis on other aspects of the material. The physical properties of the alloy, produced by mechanical alloying (MA), were characterized by x-ray diffraction (XRD) techniques, using the conventional diffractometer present in the X-ray Optics and Instrumentation Laboratory (LORXI), EXAFS measurements performed at the National Synchrotron Light Laboratory (LNLS) in Campinas, besides the techniques based on the photoacustic effect (spectroscopy and diffusivity), made in LSCM.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
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Foundations of Quantum Mechanics at UFPR

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The *Quantum and Semiclassical Theory Group* (QSTG), supported by the National Institute for Science and Technology of Quantum Information (INCT-IQ/CNPq, Brazil), is presented and its main scientific interests are enumerated. Some of our recent developments in the fields of quantum foundations and quantum information are briefly discussed.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Brief history of the graduate program in Physics - UFPR

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The graduate program in Physics (Setor de Ciências Exatas - Universidade Federal do Paraná) was created in 1983 (MSc) and 1993 (PhD). In my presentation I will outline the history of the program, from the first research activities in the department of Physics to the present days.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
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The Plasma Physics and Nonlinear Dynamics research group

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The Plasma Physics and Nonlinear Dynamics group of the Physics Department was createdd in 1991 and, since then, has played an important role in the development of the research activities and the formation of undergraduate as well as graduate students in theoretical and computational physics. I will present some of the topics in which we are currently working and also a brief historical outline of the research and teaching activities.

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(Non)Stationarity of neural networks under small-world topology

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The brain may be the most complex organ in the human body, and even nowadays there are many not answered questions about it. In this way, there are great efforts in the world for the development of researches to possible a better understanding about its, which is a fundamental object of life. The present work has the objective of studying the dynamic behavior of neural networks under weak coupling, specifically, with respect to the phase synchronization, (non)stationarity and stability. In this way, simulations of 1024 thermally sensitive neurons under the small-world regime are performed by a Hodgkin-Huxley type model also considering the system's dependence on temperature, which reproduces a bursting neural dynamic. As a tool for analysis, using just local field potential of network, we use the concepts of recurrence quantification analysis (RQA), specifically, the quantifier called determinism, which expresses ideas about the density of recurrent points in diagonal structures in the space of recurrence, once these structures are associated to the (temporal) dynamics of the system, as well as Kuramoto order parameter, which requires individual neuron information. Finally, it can be concluded that a network of 1024 thermally sensitive neurons, under small-world topology, presents anomalous synchronization, nonstationarity related to two-state intermittence and multistability for weak coupling region and for transition to synchronization, such characteristics may be associated with neuronal diseases. Regarding the methodology used, it can be concluded that the recurrence analysis (RQA) is more efficient to evaluate (non)stationarity in comparison to the Kuramoto's order parameter, besides, RQA use data of local field potential, which can be easily obtained experimentally.

I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

A qualitative look at the interplay between magnetic moment and magnetocrystalline anisotropy in tetragonally-distorted galfenol films

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[1]Universidade Federal do Paraná

[2]Institut des NanoSciences de Paris

Magnetic properties of Fe100-xGax (x = 15 and 30) epitaxial thin films on ZnSe/GaAs(001) substrates were studied experimentally and theoretically. The samples were grown by molecular beam epitaxy and adopt body centered structures with tetragonal distortion along the film normal with c/a ratio varying from 1.014 to 1.036. We studied the effects of the tetragonal distortion of Fe lattice due to the incorporation of Ga atoms on the magnetocrystalline anisotropy and the changes on the spatial-symmetry of exchange-correlation magnetic field. The experimental results were obtained through the vibrating sample magnetometer technique, and allowed us to observe a behavior given by the k1 constant for iron as measured by Reiger et al [1] and Ye et al [2] in the in-plane anisotropy. We also observed an additional anisotropy axis separated by 60° that is related to K2 iron-like constant [2]. Density functional theory calculations were performed for two different values of Ga content and shown that Fe atoms placed at first neighborhood of Ga positions present stronger distortion in the local exchange-correlation field than second neighbor Fe atoms due to significantly changes in magnetocrystalline anisotropy by addition of Ga. Magnetic contributions of Ga nearest neighbors and distortions in the local magnetic moment distribution were identified as main sources of change in the four-fold magnetocrystalline anisotropy. This behavior is enhanced from x = 15 to 30. Our current results corroborate the understanding that the magnetostrictive behavior observed in Fe100-xGax series are straightforwardly originated from their electronic properties.

Acknowledgments:

We thank LCPAD for computational support, LCNano/SisNANO, CAPES and CNPq for financial support.

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I WORKSHOP DO PROGRAMA DE PÓS-GRADUAÇÃO EM FÍSICA
21 a 23 de Março de 2018

Band gap and Drude weight in the RVO_3 series (R= Sr, Ca, La, Y) series by DTF calculations

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In this study we analyzed by Density Functional Theory (DFT) the electronic structure and optical functions of some important perovskites based on vanadium oxides. The present perovskites RVO_3 (R = Sr, Ca, La, Y) studied are final compounds of series of systems with strong electron correlation of 3*d* electrons of the transition metal (V) and the crystalline field. The metal-insulating phase transition is observed with the atomic substitution at the R site, described by the Mott-Hubbard regime. The great challenge of calculating the properties of crystalline solids using DFT is the good choice of the exchange-correlation potential ν_{xc}. Here we use a semilocal approach to such, the modified Becke-Johnson exchange potential (mBJ). The mBJ potential has the advantage of low computational cost when compared to the GW calculations and it is not necessary to add U and J constants as in the LSDA + U calculations. In addition, it shows more consistent results for insulators when compared to the LSDA and GGA approximations. The energy gap resulting from the mBJ approach provided results for DOS and optical conductivity consistent with the experimental results of other authors. It should be noted that the V 3*d* states are deployed from crystalline field on the subbands t_{2g} and e_g of majority and minority spins. The divisions observed in the DOS between the majority and minority spins were caused by the magnetic character of each compound. The metal character was defined by the Drude contribution observed in the optical functions (dielectric constants) calculated.

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Equilíbrio MHD estacionário para plasma com rotação azimutal em um sistema de coordenadas cilíndricas

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An equation for MHD stationary equilibrium of rotating plasmas in the azimuthal direction is derived in the case of an cylin-drical coordinate system with a plasma describing the plasma as an infinite-conductivity fluid, considered the entropy is a surface quantity. For the resolution of this differential equation it was necessary to propose profiles for both pressure and current flow. Firstly we did a review of the solution obtained by Maschke and Perrin, where they considered linear profiles for both pressure and current flow. Next we present two new solutions, one quadratic for current flow and pressure, one linear for pressure and quadratic for current flow. From these solutions, We plot several graphs, where we analyze the effect of rotation on the components of the magnetic field and current density, as well as the effect of the rotation on the pressure and the magnetic flux.

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On the definition of work under a microscopic perspective

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Quantum mechanics can be seen as a robust mathematical framework that describes experimental results associated with microscopic systems. On the other hand, the theory of classical thermodynamics (along with statistical physics) has been used to characterize macroscopic systems in a general way, where mean quantities are considered and the connection between them are formally described by state equations. In order to relate these theories and build up a more robust one, recently proposed works have been developed to connect the fundamental ideas of thermodynamics with microscopic quantum systems. This emerging theory is sometimes called Quantum Thermodynamics. Some key concepts associated with this recent theory are work and heat, already treated in the scope of classical thermodynamics, relating each other with the first law of thermodynamics. Alicki, in a paper published in 1979, establishes a definition for both quantities in which the first law is immediately obtained for a general quantum system: the density matrix time rate is explicitly connected with heat and the time rate of the Hamiltonian are related with work. Although these definitions have been adopted by several authors to investigate features associated with quantum systems, there is not a formal justification for relating heat only with the density matrix changes and work only with changes in the Hamiltonian. In the present work aims at investigating the definition of work in a general system. Therefore a literature review were made and is presented. A new definition for work is also proposed connecting its concept with kinetic energy changes, for classical and quantum systems. In order to analyze the new proposed form for the definition of work and compare with that proposed by Alicki, both definitions are used to evaluate the work applied on a quantum oscillator, considering the Caldirola-Kannai model. The proposed form agrees with the physical behavior expected and significant differences between it and the Alicki approach are found. Finally, the studied definitions are compared with the work calculated from an equivalent classical model, showing a direct correspondence between the presently proposed approach and the classical one.

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Nonanomalous measure of realism-based nonlocality

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Based on a recently proposed model of physical reality and an underlying criterion of nonlocality for contexts [A. L. O. Bilobran and R. M. Angelo, Europhys. Lett. 112, 40005 (2015)], we introduce a quantifier of realism-based nonlocality for bipartite quantum states, a concept that is profoundly different from Bell nonlocality. We prove that this measure reduces to entanglement for pure states, thus being free of anomalies in arbitrary dimensions, and identify the class of states with null realism-based nonlocality. Then we show that such a notion of nonlocality can be positioned in a low level within the hierarchy of quantumness quantifiers, meaning that it can occur even for separable states. These results open a different perspective for nonlocality studies.

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Calculation of transport coefficients of gaseous mixtures at low density based on ab initio potentials

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The transport coefficients for a mixture of noble gases were carried out applying the Chapman-Enskog method, applying quantum approach to the interactions between atoms. This method allows us to obtain results with a high precision expanding the velocity distribution function of the mixture under an assumption that the mixture is close to equilibrium. The ab initio potentials have been used for the intermolecular collisions of all species, which are obtained from the main principles without a necessity to adjust some parameters using experimental data. In this work, the viscosity, thermal conductivity, diffusion and thermal diffusion coefficients for the Helium-Neon mixture have been calculated, in a wide interval of the temperature and for various values of the molar fraction. Comparing the present results with those obtained by other authors, we observed that they are in agreement within the uncertainty of the corresponding works. However, the present results have the highest accuracy among all data available in the literature.

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Electronic structure of a p-d model

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The transition metal oxide family presents very interesting physical properties. For instance, high-T_C superconductivity, colossal magneto-resistance, metal-insulator transitions, etc. They are important not only in basic science, but also in technological applications. The minimal model needed to study these compounds is the so called p-d model. The p-electrons come from the oxygen (O) ligands, whereas the d-electrons arise at the transition metal (M) sites. The model includes the energy of the O 2p electrons, the energy of the M 3d electrons, the repulsion of the M 3d electrons, as well as the O 2p – M 3d hybridization. This model is a simple representation of the complex electronic structure, but allows us to gain insight about the importance of correlation effects. To this end, we solved the model using an exact diagonalization method. We present here both the static (expectation values) as well as the dynamic (spectral weight) results. The spectral weight gives the probability and energy required to remove or add an electron. s in the p or d layer. The results show that the correlation effects play a critical role in the electronic structure of this model.

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X-ray spectroscopy and extended cluster model calculations of MoO_2, RuO_2 and Rh_2O_3

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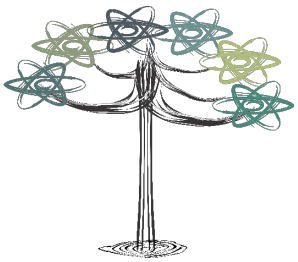
The electronic structure of 3d transition metals oxides (TMO) and its relations with the main charge fluctuations are already well established in the literature. This work investigated such relations for 4d TMO's, as well as their electronic structures. Three different 4d TMO's were studied in the present report: a distorted d^2 metal (MoO_2), a regular d^4 metal (RuO_2), and a regular d^6 insulator (Rh_2O_3). Experimental XPS and XAS spectra were obtained and compared to an extended cluster model calculation, which considers all the relevant charge fluctuations: (i) between MT 4d and O 2p ions (for all compounds), (ii) between neighboring Mo ions (dimers in its crystal structure), and (iii) the contribution of the coherent electrons (metallic character, in the molybdenum and ruthenium oxides). The results indicate a relatively high electron count in the ground state for all compounds: 3.1 (MoO_2), 5.2 (RuO_2), and 6.9 (Rh_2O_3). This can be attributed to the strong mixing between MT 4d - O 2p that is present in all cases. The predominance of a unscreened configuration in the main peak composition of Mo 3p core level spectrum indicates that it is energetically unfavorable to screen the core-level hole for MoO_2. Ru 3p and Rh 3p results shows a main peak and some satellite structures which are both screened by oxygen. Coherent screening is also present in the RuO_2 satellites. The MoO_2 and RuO_2 VB XPS results shows coherent screening at Fermi level, confirming their metallic behaviour. This is not true for Rh_2O_3 since it can be thought as d^6 band insulator due to its large value for crystal field parameter. MoO_2 and RuO_2 O 1s XAS shows two main structures splitted by the crystal field effect. The broader peak arises from O 2p - MT 4d interaction. A single asymmetric peak is showed for Rh_2O_3 and it arises from an e_g electron addition. All the presented experimental spectra of the three systems were reproduced using the same set of parameters.



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Fundamental Diagram of Traffic Flow from Prigogine-Herman Equation

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Since 1985, the Group of Phenomenological and Statistical Thermodynamics of the Federal University of Paraná develops analytical and numerical methods for the study of irreversible processes in continuous media and rarefied gases, based on usual and extended thermodynamic equations, Boltzmann kinetic equation and thermodynamic theory of fluctuations. In this oral presentation, we show how the fundamental diagram of traffic flow - i.e., a diagram that gives a relation between the traffic flux (vehicles/hour) and the traffic density (vehicles/km) - can be derived from the Prigogine-Herman-Boltzmann traffic equation.