



# **II WORKSHOP do Programa de Pós-Graduação em Física**

**LIVRO DE RESUMOS**

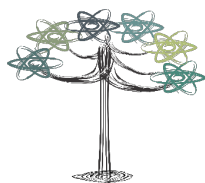
**27 e 28 de Junho de 2019**



# **II WORKSHOP do Programa de Pós-Graduação em Física**

## **LIVRO DE RESUMOS**





**II WORKSHOP DO  
PROGRAMA DE PÓS-  
GRADUAÇÃO EM  
FÍSICA**  
27 e 28 de Junho de 2019

## **Palestrantes**

Profa. Marcia Cristina Bernardes Barbosa – IF-UFRGS – Mulheres na ciência

Profa. Carla Göbel Burlamaqui de Mello – PUC-RJ – A Física de Sabores no Large Hadron Collider: Matéria vs. Antimatéria, partículas exóticas e anomalias

Prof. Osvaldo Baffa Filho – Departamento de Física – FFCLRP-USP Ribeirão Preto – Nanopartículas em Física Médica

Dr. Harry Westfahl Junior – LNLS – Sirius: a nova fonte de luz síncrotron brasileira

Dr. Daniel Kurt Lottis – IEEE Magnetics Society, Santa Clara Valley Chapter e CLSE Consulting – Armazenamento e processamento de dados: Passado, presente, futuro

Prof. Ricardo Luiz Viana – Departamento de Física-UFPR – Breve histórico do Programa de Pós-Graduação em Física da Universidade Federal do Paraná

Prof. Marlus Koehler – Departamento de Física-UFPR – Homenagem ao Professor Ivo Alexandre Hümmelgen

Prof. José Pedro Mansueto Serbena – Departamento de Física-UFPR – Homenagem ao Professor Ivo Alexandre Hümmelgen

Profa. Alessandra de Souza Barbosa – Departamento de Física-UFPR – Positron collisions with targets of biological and technological relevance

Prof. Emerson Cristiano Barbano – Departamento de Física-UFPR – Processos ópticos não lineares induzidos por pulsos de femtosegundos

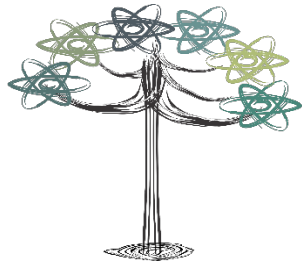
Prof. Ismael André Heisler – Departamento de Física-UFPR – Fundamentals and Applications of Multidimensional Ultrafast Spectroscopy

Prof. Giovani Vasconcelos – Departamento de Física-UFPR – Teoria H: Uma Descrição Unificada para Fenômenos de Flutuação – de Turbulência a Lasers Aleatórios “and Beyond”

Prof. Cristiano Francisco Woellner – Departamento de Física-UFPR – Materials Design through reactive molecular dynamics techniques

Prof. Thiago de Lima Prado – Departamento de Física-UFPR – Transições em redes complexas neuronais analisadas por microestados de recorrências

27/06	28/06
08:30 – Abertura	09:00 – Prof. Osvaldo Baffa Filho
09:00 – Prof. Ricardo Luiz Viana	10:00 – Dr. Daniel Kurt Lottis
09:45 – Profs. Marlus Koehler e José Pedro Mansueto Serbena	10:30 – Café
10:30 – Café	11:00 – Prof. Cristiano Francisco Woellner
11:00 – Prof. Emerson Cristiano Barbano	11:30 – Prof. Thiago de Lima Prado
11:30 – Prof. Ismael André Heisler	12:00 – Almoço
12:00 – Almoço	14:00 – Profa. Carla Göbel Burlamaqui de Mello
14:00 – Profa. Alessandra de Souza Barbosa	15:00 – Dr. Harry Westfahl Junior
14:30 – Prof. Giovani Vasconcelos	16:00 – Plenária de Encerramento
15:00 – Profa. Marcia Cristina Bernardes Barbosa	
16:00 – Café + Pôsteres	



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

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### **A negative result for Bethe Ansatz-like solutions for 2 quantum particles in a 1D box**

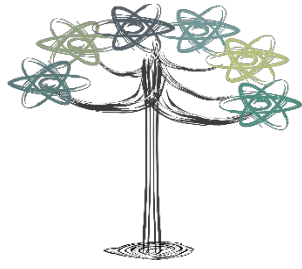
Adam Luiz de Azevedo<sup>1</sup>, Marcos G. E. da Luz<sup>2</sup>

<sup>1</sup> UFPR

<sup>2</sup> UFPR

The system composed by two interacting particles confined in a 1D region represent one the simplest situations to study dynamical properties related to classical and quantum integrability. In particular, in this contribution, we address to the quantum system composed by 2 particles in a 1D infinite box interacting by zero-range potential  $V(x_1, x_2) = \lambda \delta(x_1 - x_2)$ , where  $\lambda$  is the strength of potential. This system is equivalent to a rectangle billiard containing an only unity mass particle, in which its diagonal represents the interaction potential. The classical description of the system shows a finite number of momenta is generated when the  $\theta$  parameter associated to the ratio mass  $\gamma$  of the particles is a rational number. This one is a starting point to investigate the quantum integrability. To do this, we search for a Bethe Ansatz-like, which consists of assuming that the wave function is a finite superposition of plane waves. If this hypothesis is true, then the quantum-mechanical system is integrable. In our contribution we show the inconsistency of the Bethe Ansatz-like solutions for all mass ratio  $\gamma$ , including even the classically integrable case  $\gamma=3$ , via geometric and topological properties of the physical system. This is due to the absence of reflection symmetry, a necessary condition for Bethe Ansatz-like solutions.





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### Control Synchronization in Scale-free Neuronal Networks

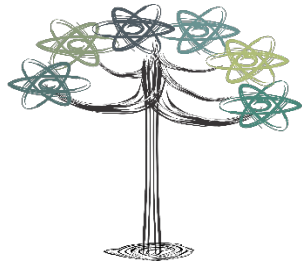
Reis, A. S<sup>1</sup>, Viana, R. L. V<sup>1</sup>

<sup>1</sup> *Universidade Federal do Paraná.*

One of the main constituents of the nervous system are the neurons. They are connected to each other in a complex way, forming a complex network of connections. In this research, will be presented a building model to a neuronal network based on human cerebral cortex, using a real connectivity matrix, obtained through experimental methods. The study of the construction of the neuronal model will be done using a network of networks, in such a way that connections in each region of the cerebral cortex can be described by a model of scale-free networks. The cortical networks will be connected to each other according to the type of synapse present in each region, and the neuronal dynamics will be studied through the two-dimensional coupled Rulkov map

$$x_{n+1} = \frac{\alpha}{1+x_n^2} + y_n + C_i$$
$$y_{n+1} = y_n - \sigma(x_n - \rho),$$

where  $C_i$  is a coupling term. Due the individuality of each neuron, they perform their activities in different rhythms so that at first there is no synchronization in their bursts. To study synchronization in the neural network, an external signal was applied on Rulkov's map so that all neurons could start a bursts at the same time. Neuronal synchronization, in general, refers to the presence of some neurodegenerative disease. In this sense, the synchronization suppression technique was employed through the application of a delay field in the neural network. It has been found that the method chosen for the suppression control is efficient to suppress synchronization when the control parameter and the delay time are set appropriately.



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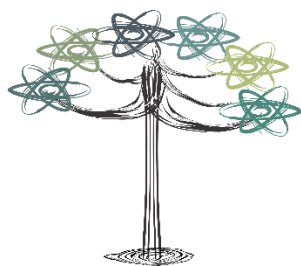
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### **Nonlocality, quantum correlations, and irrealism in the dynamics of two quantum walkers**

Alexandre C. Orthey Jr.<sup>1</sup>, R. M. Angelo<sup>1</sup>.

<sup>1</sup> *Departament of Physics, Federal University of Paraná, Curitiba, Brazil.*

That quantum correlations can be generated over time between the spin and the position of a quantum walker is indisputable. The creation of bipartite entanglement has also been reported for two-walker systems. In this scenario, however, since the global state lies in a fourpartite Hilbert space, the question arises as to whether genuine multipartite entanglement may develop in time. Also, since the spatial degrees of freedom can be viewed as a noisy channel for the two-spin part, one may wonder how other nonclassical aspects (quantumnesses), such as Bell nonlocality, Einstein-Podolsky-Rosen steering, quantum discord, and symmetrical quantum discord, evolve in time during the walk. The scarcity of such a broader investigation is possibly due to computational difficulties associated with the recursive nature of quantum walks. Here, we work around this issue by introducing a simplified Gaussian model which proves to be very accurate within a given domain and powerful for the analytical studies. Then, for an instance involving two noninteracting quantum walkers, whose spins start in the singlet state, we quantify the aforementioned quantumnesses as a function of time, and evaluate violations of both realism and related aspects of locality. In addition, we analyze situations in which the initial two-spin state is affected by white noise. The typical scenario found is such that while genuine fourpartite entanglement increases over time, all the investigated quantumnesses vanish (suddenly or asymptotically) except realism-based nonlocality. Moreover, realism is prevented for all finite times.



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### **Organic WORM memory with carbon nanoparticle/epoxy active layer**

Andressa Toppel<sup>1</sup>, Celso de Araujo Duarte<sup>1,2</sup>, Messai Adenew Mamo<sup>3,4</sup>

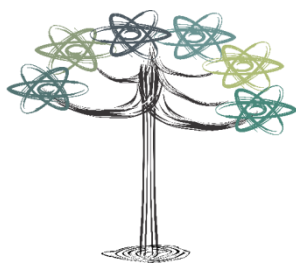
<sup>1</sup>*Programa de Pós-Graduação em Física Universidade Federal do Paraná, Curitiba, PR, Brazil*

<sup>2</sup>*Departamento de Física, Universidade Federal do Paraná, Curitiba, PR, Brazil*

<sup>3</sup>*Department of Applied Chemistry, University of Johannesburg, Doornfontein, South Africa*

<sup>4</sup>*DST-NRF Centre of Excellence in Strong Materials (CoE-SM), Johannesburg, South Africa*

Following the “All With One (AW1)” technology proposed in our earlier work, the present study is focused on the production and the characterization of write once read many (WORM) memory devices with a carbon nanoparticle/epoxy resin nanocomposite, where the main advantage stands on the ease of production of the nanostructured phase. The results revealed that short 100-ns, low-voltage (5.0-V) electric pulses are enough to record a bit, and the bit one to bit zero current state ratio  $I_{ON}/I_{OFF}$  reaches  $10^7$ .



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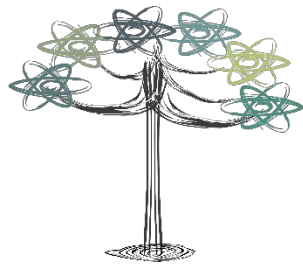
## **Study of Interaction of Small Molecules with Character of donor and acceptor on Internal Charge Transfer.**

Anne Beatriz R. Abreu<sup>1</sup>, Marlus Koehler<sup>1</sup>.

<sup>1</sup> *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 extensively 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. The combination of distinct chemical groups allows the control of the material gap. The ionization potential is related to the HOMO (highest occupied molecular orbital) energy level and the electron affinity is related to the LUMO (lowest unoccupied molecular orbital) energy level. Thus, the energy levels of the material resulting from the combination of the donor material and the acceptor material present different characteristics, with the HOMO energy level prevailing in the donor unit group and the LUMO energy level prevailing in the acceptor unit group. The difference between HOMO and LUMO provides the band gap region. We are especially interested in the investigation of the effect of the internal charge transfer (ICT) in small molecules. The computational method [1] employed to investigate the charge transfer involves as fragment analysis to quantify the coupling between molecular orbitals. In this work we investigated theoretically the variations in the ICT produced by the introduction of a larger atom in molecules formed by a combination in the donor (D) moiety and an acceptor moiety (A). Those model molecules are represented by F-(T)<sub>n</sub>, where F = fluorene, silafluorene and germafluorene whereas T is the thiophene. In the literature F has been described as an acceptor group whereas T are considered as the donor moiety. Yet our calculations indicate exactly the opposite. In addition our preliminary results indicate that there is an increase in the charge transfer when a larger atom is inserted in the F part of the molecule that has a predominantly donor character. Finally we observed a saturation in the ICT with the increase in the number of thiophenes (that shows an acceptor character in those molecules).

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



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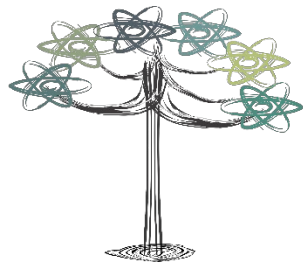
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### **Semiclassical Entanglement Dynamics for Long Times**

Arlans Juan Smokovicz de Lara, Alexandre Dias Ribeiro

*Universidade Federal do Paraná*

The entanglement phenomenon is widely considered as a pure quantum effect. However, there are several attempts to describe this characteristic using classical quantities. In particular, in our work, we are interested in the entanglement dynamics of a pure, bipartite system, initially in a product of coherent states, governed by a generic Hamiltonian. In this scenario, the linear entropy for the reduced state, a function that quantifies entanglement, can be rewritten, for short times, in terms of *real* trajectories of the equivalent classical dynamics. We show that it is possible to include *complex* trajectories in the calculation, which can contribute to improve that approximation, extending its accuracy for longer times. We also show, for a particular Hamiltonian, a first application of the obtained formula.



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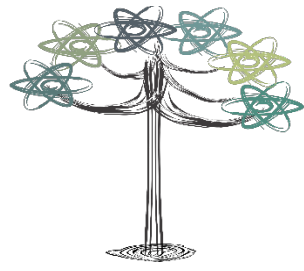
### Two qubits controlled under distinct noises

*G. J. Delben <sup>2</sup>, A. L. O. dos Santos <sup>1</sup> and M. G. E. da Luz <sup>1</sup>*

*<sup>1</sup> Universidade Federal do Paraná, C.P. 19044, 81531-980 Curitiba-PR, Brazil.*

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Realistic quantum systems are very sensitive to the surrounding environment, as a consequence their characteristic features tend to disappear quickly. The manipulation and control of quantum systems involves very subtle procedures, since the inevitable interaction with the environment occurs that leads to a loss of information that causes transformation of the quantum superposition into statistical mixtures, a process called decoherence and disappearance of quantum entanglement in composite systems. That said, in this work we extend the piecewise time-independent control to a composite system formed by two qubits in X state. In order, to model the system we use the Lindblad equation for two different dissipative interactions, amplitude damping and phase damping. The quantum measures studied are decoherence and entanglement of the system. For this we calculate the measures of fidelity and concurrence. We compared different control objectives, such as population control of the excited state, population of the off diagonal terms and objectives directly related to entanglement - possible analytically for systems in X state. We characterize the revival and the sudden death of the entanglement. We study the relationship between control and the time the system remains entangled. We present the response of the system to the external field under the effect of the two different dissipative interactions, which are different. The control method is effective and a excellent option, because it is mathematically simple, computationally fast and physically intuitive - because we can identify the terms of the density matrix directly affected by the external field.



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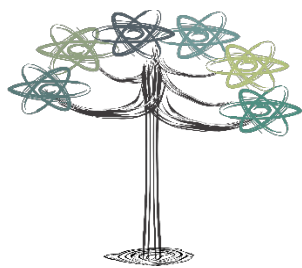
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### **A mechanism for explosive synchronization of neural networks**

B. R. R. Boaretto<sup>1</sup>, R. C. Budzinski<sup>1</sup>, T. L. Prado<sup>1</sup>, S. R. Lopes<sup>1</sup>

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Explosive synchronization (ES) has recently been observed in complex networks with chaotic oscillators when there is a frequency-degree correlation. It is also known that ES is verified in heterogeneous networks which feature a disassortative property. Here, we explore the explosive synchronization transition in a complex neural network composed of non-identical two-dimensional maps. We use the Newman-Watts route to obtain the coupling matrix of the network, starting with a regular one and adding shortcuts with a given probability. We find a range of probabilities in which the network displays an abrupt transition characterizing an ES accompanied by the appearance of hysteresis on the network dynamics. It is shown that this transition from a chaotic non-synchronized asymptotic state to a regular behavior synchronized state is induced by a frontier crisis as the coupling parameter is raised and, on the other hand, the synchronized regular state loses stability by a traditional saddle node bifurcation as the coupling parameter is decreased configuring the hysteresis loop.



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### ESTRUTURA ELETRÔNICA DO COMPOSTO SUPERCONDUTOR $\text{SrTiO}_{3-6}$

Carlos Alberto Martins Junior<sup>1</sup>, Dr. Rodrigo José Ochekoski Mossanek<sup>1</sup>

<sup>1</sup> Universidade Federal do Paraná.

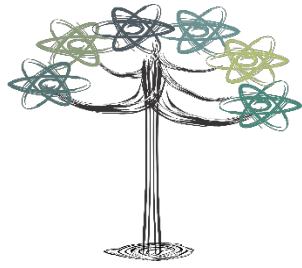
O composto não-estequiométrico  $\text{SrTiO}_{3-6}$  apresenta diversas propriedades físicas interessantes originadas na estrutura eletrônica, dentre elas, podemos citar a supercondutividade a baixa temperatura [1], grande permissividade elétrica [2], além de, diferentemente da contraparte estequiométrica, ser caracterizado como condutor [1] e apresentar ordenamento magnético [3]. A fim de compreender a origem dessas propriedades, foram feitas medidas de fotoemissão (PES) e de fotoemissão ressonante (RPES) na borda  $L_3$  do Ti em monocristais de  $\text{SrTiO}_{3-6}$  no limite de baixa concentração das vacâncias. Ambas as medidas foram realizadas em temperatura ambiente, sendo que foram selecionadas energias dos fótons de 103 eV, para PES, e de cerca de 450 eV, para RPES. Além dessas medidas, foram realizados cálculos de estrutura de bandas, usando DFT com aproximação GGA, em uma série de sistemas STO não-estequiométricos, todos no limite de concentração de vacâncias diluídas. Os resultados do PES mostram que a banda de valência é sensível a concentração de vacâncias, e que para um alto nível de concentração vacâncias existe uma anisotropia nas ligações químicas. A partir dos RPES, foi possível verificar que existe hibridização do Ti 3d com O 2p, e que essa ligação também é afetada pela concentração de vacâncias. Os cálculos mostram que a introdução de vacância de oxigênio gera uma assimetria na ligação Ti-O nos átomos próximos a vacância.

[1] N. Shanthi and D. D. Sarma, Electronic Structure of Electron Doped  $\text{SrTiO}_3$ :  $\text{SrTiO}_{3-d}$  and  $\text{Sr}_{1-x}\text{La}_x\text{TiO}_3$ , Physical Review B Volume 57, Number 4 (1998).

[2] Weaver, H, Dielectric Properties of Single Crystals of  $\text{SrTiO}_3$  at Low Temperatures H. E. Weaver, J. Phys. Chemistry of Solids, (1959)

[3] Yongjia Zhang, Jifan Hu n , Ensi Cao, Li Sun, Hongwei Qin, Vacancy induced magnetism in  $\text{SrTiO}_3$ , Journal of Magnetism and Magnetic Materials, 324, 2012.





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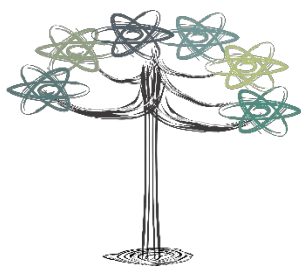
### Vetores de Lyapunov em Sistemas de Alta Dimensão

Carolini Costa Felicio<sup>1</sup>, Marcus Werner Beims<sup>2</sup>.

<sup>1</sup> *Universidade Federal do Paraná.*

<sup>2</sup> *Universidade Federal do Paraná.*

Prever eventos extremos é um problema que atrai atenção em várias áreas. Considerando um evento extremo como um pico na série temporal de um observável do sistema, estamos interessados na predição de tal acontecimento. O cálculo teórico dos vetores de Lyapunov, que são vetores que apontam na direção das variedades estáveis e/ou instáveis no espaço tangente, foi proposto dez anos atrás. Algumas aplicações para os vetores de Lyapunov são o estudo do efeito "grude" (stickiness) próximo às regiões de não hiperbolicidade do espaço de fases, origem de buracos em torus de sistemas conservativos e previsão de picos em sistemas caóticos. O objetivo deste trabalho é analisar a possibilidade de prever picos em sistemas de alta dimensão e para isto utilizamos os modelos generalizados de Lorenz, sendo estes os chamados Lorenz 5D e Lorenz 6D. Para predizer o aparecimento destes picos estamos estudando o alinhamento dos vetores de Lyapunov ao longo do fluxo.



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### Monte Carlo simulations of organic photovoltaic devices

C. A. M. Moraes<sup>1</sup>, J. A. Govatski<sup>1</sup>, M. Koehler<sup>1</sup>

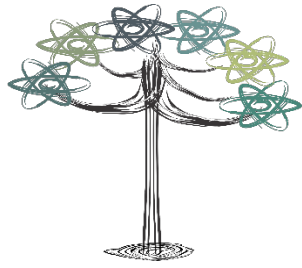
<sup>1</sup> *Universidade Federal do Paraná*

Organic photovoltaic devices offer some advantages over inorganic panels. The manufacturing process is simplified and cheap, since the flexibility derived from the organic semiconductors allows the manufacture of tens of meters of solar cells. In addition, the synthesis of synthetic polymers allows the manipulation of physical and electrical properties through the modification of the atomic chain. However, the efficiency of these devices still borders 50% of an inorganic solar panel. They are composed predominantly of conjugated polymers, i.e., polymers having in their chain the intercalation of single and double bonds between the carbon atoms. From this intercalation arise the  $\pi$ -bonds, which comprise energy levels corresponding to the visible spectrum of light. In these semiconductors occurs the generation of an exciton: one electron and hole connected by coulomb force. The free charges that compose the current of the device come from the dissociation of the exciton, a process that is still object of study and responsible for the low efficiency[1,2]. In this context, the present work offers a computational approach using the Monte Carlo Kinetic method for the study of organic photovoltaic cells. Based on the BKL algorithm[3] and the composition proposed by Casalegno[4], the material is represented by sites and each physical phenomenon has an associated rate; a list with all possible events is established followed by the linking of the respective probabilities of occurrence through the generation of random numbers. Through this construction it is possible to obtain the characteristic JxV curve and to verify the influence that the interface between the donor and acceptor materials and rates such as hopping, the creation and dissociation of excitons have for the efficiency of the device. Several simulations were performed considering different types of interface between materials, from flat to extremely rough. It has been found that rough interfaces present a higher short circuit current at the cost of a lower open circuit voltage.

**Acknowledgments:** The authors thank CAPES for their financial support and the physics post-graduation program of UFPR.

#### References:

- [1] M. R. Narayan and J. Singh, *Journal of Applied Physics* 114:7 (2013)
- [2] J. H. Yap, T. T. To, S. Adams, *Journal of Polymer Science* 53: 270-279 (2015)
- [3] A. B. Bortz, M. H. Kalos and J. L. Lebowitz, *Journal of Computational Physics* 17:10-18 (1975)
- [4] M. Casalegno, G. Raos and R. Po, *The Journal of Chemical Physics* 132:9(2010)



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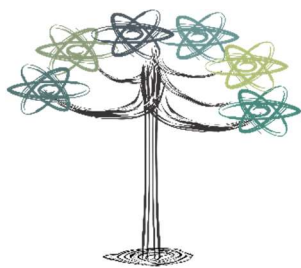
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### **Tripartite realism-based quantum nonlocality**

D. M. Fucci<sup>1</sup>, R. M. Angelo<sup>1</sup>

<sup>1</sup> *Department of Physics, Federal University of Paraná, P.O. Box 19044, 81531-980 Curitiba, Paraná, Brazil*

A concept of context nonlocality defined from an operational criterion of physical reality was recently used to define a realism-based nonlocality quantifier for bipartite quantum states. Taking into account that multipartite states are known to display features that are absent in bipartite states, we take a step further and introduce a realism-based nonlocality quantifier for tripartite states. This measure reduces to genuine tripartite entanglement for a certain kind of pure tripartite state and manifests itself in correlated mixed states even when measures of quantum correlations vanish. Then, we conduct a case study for noisy GHZ and W states and investigate monogamy properties, finding that the realism-based nonlocality for tripartite states is monogamous for noisy GHZ states and non-monogamous for noisy W states.



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### **Photothermal effect in conjugated polymers/fullerene heterojunctions nanoparticles**

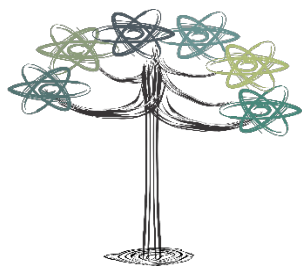
Deize Corradi Grodniski<sup>1</sup>, Kaike Rosivan Maia Pacheco<sup>1</sup>, Maiara de Jesus Bassi<sup>1</sup>,  
Lucimara Stolz Roman<sup>1</sup>, Marlus Koehler<sup>1</sup>

<sup>1</sup> *Federal University of Paraná - UFPR.*

The non-radiative recombination is one of the most important electronic processes in semiconductors devices. In organic solar cells, the excitons generated from light excitations in the interface between the donor and acceptor materials can dissociate into free charges or, then, recombine nonradiatively.

The latter is one of the factors that represent losses in the efficiency of these devices. What is known, is that non-radiative decays are dissipated as thermal energy into the medium. In the field of biomedicine, the process of generating heat by light excitation in conjugated polymers is already used as a complementary treatment against cancer, known as photothermal therapy.

In this work, our objective is to study and understand how the presence of fullerene in donor/acceptor heterojunctions favors non-radiative recombinations and also the processes involved for these recombination to happen. The temperature variations in nanoparticles of heterojunctions of the conjugated polymer poly(3-hexylthiophene-2,5-diyl) - P3HT - and the fullerene [6,6]-phenyl-C71 methyl-ester-butyric-acid - PC71BM and also the heterojunction of the conjugated polymer Poly[2,7-(9,9-dioctyl-dibenzosilole)-alt-4,7-bis(thiophen-2-yl)benzo-2,1,3-thiadiazole] – PSIF-DBT and the fullerene PC71BM, were measured from the incidence of a laser.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

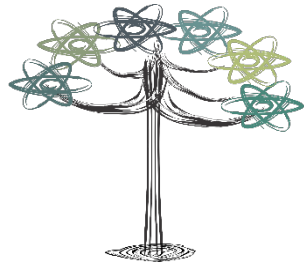
27 e 28 de Junho de 2019

### **Band structure and cluster model calculations of $\text{LaNiO}_3$ compound to photoemission, O 1s X-ray absorption, and optical absorption spectra**

E. Alves<sup>1</sup>, H.P. Martins<sup>1</sup>, S. Domenech<sup>1</sup>, M. Abbate<sup>1</sup>

<sup>1</sup> *Universidade Federal do Paraná (UFPR).*

We studied the electronic structure of  $\text{LaNiO}_3$  using band structure and cluster model calculations. This compound is a paramagnetic metal with a R3c rhombohedral structure. The band structure was calculated using the generalized gradient approximation (GGA). The cluster model was solved using the configuration interactions (CI) many-body method. We present results for the density of states (DOS), the spectral weight, and the dielectric function  $\epsilon_2$ . The calculations are compared to previous photoemission (PES), O 1s X-ray absorption (XAS), as well as optical absorption spectra. Both band structure and cluster model results are in good agreement with the experimental data. We point out that this concordance is very rare and far from trivial; we argue that this may be due to the unusual characteristics of the ground state of  $\text{LaNiO}_3$ .



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### Scattering map for a binary system of strong gravitational field black holes

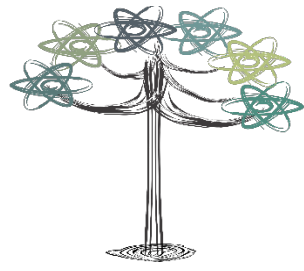
Edson E. S. Filho<sup>1</sup>, Amanda C. Mathies<sup>1</sup>, Ricardo L. Viana<sup>1</sup>

<sup>1</sup> *Universidade Federal do Paraná.*

At the current days the study of black holes are very popular, the finding of gravitational waves by a binary system, the first picture of a supermassive black hole, with this new light of black hole we propose to study the movement of photons around a system of two black holes set apart by a certain distance where one black hole does not influence the other, so the motion of light rays in the neighborhood of one black hole can be considered to be the result of the action of each black hole separately. Using this approximation, the dynamics is reduced to a two-dimension map.

As is known there are four main types of black holes, Schwarzschild (static and characterized by its mass), Reissner-Nordstrom (static, characterized by mass and charge), Kerr (with angular momentum) and Kerr-Newman (with angular momentum and charge), as the last two are very hard to be analysed, we choose to do the study on Reissner-Nordstrom, having in mind that when the charge goes to zero the system falls on Schwarzschild.

First step was to get to the equation that describes the movement around one of the black holes, following by iterating the map, we found that the map is chaotic, with fractal basin boundary separating the possible outcomes (escape or falling into one of the black holes), going forward we used the box-counting dimension and the entropy to confirm the fractal characteristics of the map.



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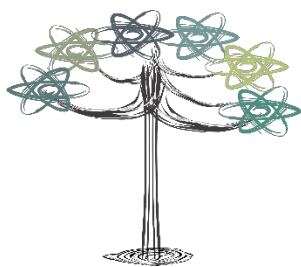
27 e 28 de Junho de 2019

### Prediction methods applied to chaotic systems

Eduardo Luís Brugnago<sup>1</sup>, Marcus Werner Beims<sup>1</sup>

<sup>1</sup> *Universidade Federal do Paraná*

Interested in predicting the behavior of chaotic systems, we propose methods of classification and apply machine learning techniques to chaotic time series. Also, we successfully use computational techniques to determine the angles between the unstable varietie and the direction of flow in the Lorenz system. Our main results are the forecast of the end of the current seasons and the duration of the coming seasons. A comparison between the methods, considering the precision in the results and the applicability of those, evidences the superiority of the machine learning techniques.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

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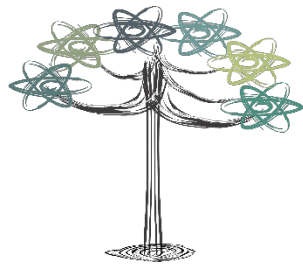
### Photovoltaic Devices Based on Metal Oxides Heterostructures

MOURA, E. A.<sup>1</sup>, SERBENA, J. P. M.<sup>1</sup>

<sup>1</sup> *Universidade Federal do Paraná, Departamento de Física.*

Photovoltaic power generation systems are in great expansion. In the last 10 years, photovoltaic power generation has increased from 21 TWh to 584 TWh in the world. However, in most places, these systems still can not compete in terms of costs with the electricity generated by conventional generation systems. Currently, many efforts are being devoted to the search for new materials with favorable properties for photovoltaic and, mainly, low cost applications. In this context, the semiconductor metal oxides appear as an attractive and promising alternative to the photovoltaic application due to its abundance, chemical stability and many of them are non-toxic, in addition, it is possible to obtain them using simple and inexpensive synthesis techniques. These factors are fundamental for the reduction of the manufacturing costs of the photovoltaic modules (solar cells) and consequently, the reduction of the kWh price of generated photovoltaic energy. Metal oxides are already widely used in photovoltaic devices as transparent conducting electrodes or as an electron/hole carrier layer. However, photovoltaic devices based entirely on metal oxides is something that is attracting interest in recent years. Although most oxides have a broad band gap in the region of the visible spectrum, cuprous oxide ( $\text{Cu}_2\text{O}$ ) has a high potential for application in photovoltaic device as a light absorber, due to its high light absorption coefficient in the order of  $10^5 \text{ cm}^{-1}$  with a direct optical band gap between 2.0 and 2.2 eV. In this perspective, we are preparing and characterizing photovoltaic devices based entirely on metal oxides at the pn junction, formed by a thin layer of nickel oxide (hole-carrying layer), a layer of cuprous oxide (active layer) and a layer of oxide of zinc, using ITO (Indium Tin Oxide) and aluminum electrodes. The metal oxides used to prepare the devices were obtained by sol-gel process and deposited by spin coating. Preliminary results of the photovoltaic characterization of the devices show an energy conversion efficiency ( $\eta$ ) of 0.1 % with a short-circuit current density ( $J_{sc}$ ) of  $0.62 \text{ mA.cm}^{-2}$  and an voltage open-circuit ( $V_{oc}$ ) of 0.34V.





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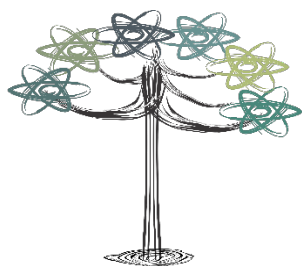
27 e 28 de Junho de 2019

### **Families of quantum states of right triangle billiards**

F. Teston, F. M. Zanetti, M. G. E. da Luz

*Federal University of Paraná*

The purpose of this work is to analyze the behavior of the quantum solutions for the right triangular billiard with variable geometry in the region of transition between the regular and chaotic solutions for the classical case, being the modifications in the geometry caused by the variation of its internal angles  $\beta$ . The method used to obtain the solutions is the boundary wall method (BWM), a quantum scattering method whose main ingredient is the T-matrix, which carries information about the geometry and energy  $E = k^2$  of the billiards. Using the properties of the T-matrix, we can obtain the billiard spectrum as a function of its geometric parameters  $\beta$  and then determine the dynamics of the families of eigenstates resulting from these variations in parameter space  $k \times \beta$ . By analyzing the wave functions associated with these eigenstates, we obtain information about certain behaviors, such as the repulsion among families. It is also carried out an analysis of how these observations properties relate to the billiards genus. In fact, it is well known in the classical case that the internal angles (determining the system genus) are associated with the billiard regularity. Therefore, from these results we try to connect the quantum chaology of the right billiard with topologic properties, the genus, associated with then non-integrability of the classical case.



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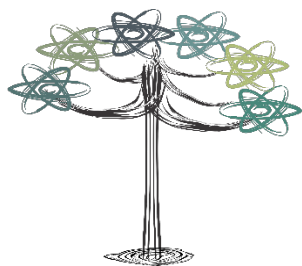
27 e 28 de Junho de 2019

### **Characterizing the transient dynamics towards stationary Lévy reaction-diffusion process**

F. R. Rusch.<sup>1</sup>, M. G. E. da Luz<sup>1</sup>.

<sup>1</sup> *Universidade Federal do Paraná.*

In random search models, the landscape environment plays, of course, a fundamental role. Usually, many runs for the same set of search parameters are made (for different randomly created landscapes) so to obtain a large enough sample of realizations for proper statistical analysis. The number of total targets remains constant, although its spatial distribution changes at each new simulation. In this work, we present an analytical model to describe the dynamics of the search process considering a changing environment. The goal is to characterize transients features in a foraging process considering Lévy search strategies. For so, we assume that the density of resources in the search environment increases at a constant rate in time. Through two processes, creation for targets and annihilation (by finding them), we study the foraging efficiency as well as the emergent features of the environment. We show that for the search strategy  $\mu = 1.0$ , our analytical model (through a mean-field approximation MFA) provides a very good solution compared to the numerical simulations. As the parameter  $\mu$  changes toward the diffusive limit of  $\mu = 3.0$ , the discrepancy between the MFA and the numerics increases. As the most important properties of the search dynamics, we determine the evolution in time of quantities such as available targets in the environment, the number of detected targets, and search efficiency. We also elucidates at each condition the system finally evolves to the steady state after going through the transient period.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **Espectro de ressonância de forma do ácido acrílico**

Francisco Fernandes Frighetto<sup>1</sup>, Márcio Henrique Franco Bettega<sup>1</sup>

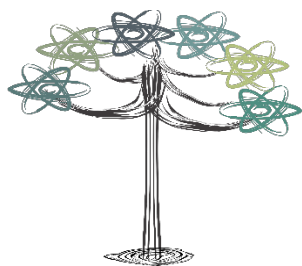
<sup>1</sup> *Departamento de Física, Universidade Federal do Paraná*

O ácido acrílico ( $C_3H_4O_2$ ), o mais simples dos ácidos carboxílicos insaturados, tem papel importante na produção de materiais (como plásticos) e na medicina. Além disso, a presença de compostos acrílicos (como a acrilonitrila) no meio interestelar fornece mais uma razão pela qual se torna interessante estudar o ácido acrílico, uma vez que os compostos acrílicos são formados com base no ácido acrílico.

Também vale comentar que não foram identificados dados teóricos e experimentais relativos à seção de choque de espalhamento do ácido acrílico. Desta forma, o principal objetivo deste trabalho é o de propor e analisar a seção de choque de espalhamento elástico de elétrons do ácido acrílico em suas conformações s-cis e s-trans.

Como o ácido acrílico contém um grupo vinil ligado a um grupo carboxílico, também se torna interessante comparar sua seção de choque com a seção de choque do etileno ( $C_2H_4$ ) e do ácido fórmico ( $CH_2O_2$ ) em busca de semelhanças.

Os cálculos realizados para se obter as seções de choque utilizaram o método multicanal de Schwinger, implementado com pseudopotenciais, nas aproximações estático-troca e estático-troca-polarização.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### Low-energy electron scattering by the thiophene molecule: a study about the effect of polarization on the electronic excitation

Giseli M. Moreira<sup>1</sup>, Fabris Kossoski<sup>2</sup>, Márcio H. F. Bettega<sup>1</sup>, and Romarly F. da Costa<sup>3</sup>.

<sup>1</sup> Universidade Federal do Paraná.

<sup>2</sup> Aix-Marseille Université.

<sup>3</sup> Universidade Federal do ABC.

Thiophene is a heterocyclic compound, which has a sulfur atom bound to four carbon atoms. In addition to being a prototype of biological interest, thiophene has important technological applications such as in semiconductors, solar cells, diodes, transistors, and others [1,2]. For many of these applications, it is of fundamental importance to obtain the data of the cross sections, electronic structure and spectroscopy of this system. Within the context discussed above, we apply the Schwinger multichannel method implemented with norm-conserving pseudopotentials (SMCPP) [4] to study the influence of polarization effects on the electronic excitation of the thiophene molecule by low-energy electron impact. The description of the multichannel coupling effects and the strategy used for the composition of the coupled channel space were obtained according to the minimal orbital basis for single configuration interactions (MOB-SCI) approach [3]. In particular, for this study, the choice of the hole-particle pairs that compose the active space of single-excitations was made in order to provide a good description of the lowest triplet state that is, in order to properly describe the electronic transition  $^1A_1 \rightarrow ^3B_2$ . In our calculations, the  $^3B_2$  state opens at the energy 3.41 eV, which is in good agreement with previous work reported in the literature [5,6]. We aim to investigate if the inclusion of polarization effects has the same influence on the electronic excitation cross section, as the one already reported by da Costa *et al.* [7,8] for electron collisions with ethylene and furan. We present results of integral and differential elastic and electronically inelastic cross sections for energies ranging from 0 to 15 eV. We compare our results with the recent work of Loupas *et al.* [6], which reports data from calculated and measured cross sections for the thiophene molecule.

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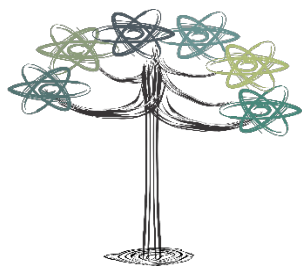
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## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

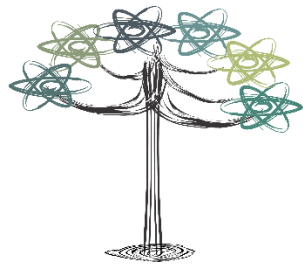
27 e 28 de Junho de 2019

### **Cr<sub>2</sub>N nanoparticles synthesized by pulsed laser irradiation**

Greici Gubert, Ronei Cardoso de Oliveira, Daniel da Silva Costa, *Gabriel* Kavilhuka Metzger, Irineu Mazzaro, Guinther Kellermann, Evaldo Ribeiro, José Varalda and Dante Homero Mosca

*Universidade Federal do Paraná, Centro Politécnico, 81531-980 Curitiba, Paraná, Brazil.*

Chromium nitride nanoparticles with cylindrical shapes having aspect (height-to-diameter) ratio with particle size (mean diameter) distribution between 0.8 nm and 30 nm were produced by laser irradiation of a chromium target immersed in liquid nitrogen. The Cr was directly converted to chromium nitrides nanoparticles according to selected-area electron diffraction analyses using transmission electron microscopy technique. Crystalline nanoparticles are mostly consisting of Cr<sub>2</sub>N without evidence of core-shell structure which is commonly reported together with conversion of Cr<sub>2</sub>N to CrN and mixture of chromium oxides. In addition, there is no evidence of oxidation by storage or photodegradation of the nanoparticles in isopropyl alcohol suspensions. The intensity profile of small-angle X-ray scattering indicate that geometrical shape of the nanoparticles is not spherical, but cylindrical with an aspect (height-to-diameter) ratio in the proportion 7:10. UV-Vis absorption spectroscopy reveal presence of surface plasmon absorption at ultraviolet region at wavelengths of 350, 372 and 397 nm. First-principles calculations of density of states, dielectric function, and optical conductivity performed within the theoretical framework of density functional theory for Cr<sub>2</sub>N with hexagonal structure corroborate the formation of surface plasmons.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### Trojan Quantum Walks: A brief explanation

Henrique Sobrinho Ghizoni<sup>1</sup>, Edgard Pacheco Moreira Amorim<sup>2</sup>

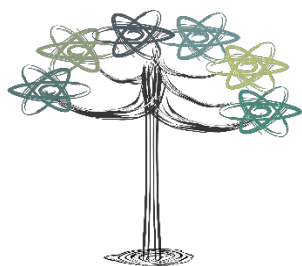
<sup>1</sup> *Universidade Federal do Paraná-UFPR*

<sup>2</sup> *Universidade do Estado de Santa Catarina-UDESC*

Quantum walks are the quantum analogue of the classical random walks, it have been widely studied as quantum search algorithms and a way to perform universal computation. The quantum walker is a spin-1/2 particle positioned over discrete positions in a one-dimensional lattice. The main features of quantum walks are the ballistic dispersion being quadratically superior over their classical counterparts and the creation of entanglement between the spin and position.

From the epic poem, the term "Trojan" was used to name a group of asteroids which share the Jupiter's orbit around the Sun. The center of mass of the Trojan asteroids is steady relative to Jupiter, once they are trapped on stable Lagrange regions (L4 and L5) of this celestial mechanical system. In the quantum-mechanical context, Trojan wave packets have non-spreading and non-stationary behavior and they have been observed as a localized Rydberg electron over a circular orbit with dispersion suppressed by external fields

We studied one-dimensional quantum walks starting from two kinds of initial position states (local and Gaussian) with a NOT gate on a specific position, which promotes a chiral reflection of the state. In summary, we have performed some numerical calculations which show that quantum walks can also exhibit a non-spreading and non-stationary behavior. When quantum walks start from a Gaussian state with a large enough initial dispersion, they time-evolve with only two opposite peaks without considerable amplitudes of probability between them. After one of the peaks is reflected by a NOT gate on a particular position, the relative velocity between peaks vanishes creating a double-peak Trojan wave packet without quantum correlation (entanglement) between internal and external degrees of freedom. We hope our findings can be used to foster the discussion about the quantum-classical limits of such walks and the experimental researchers can corroborate our results.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

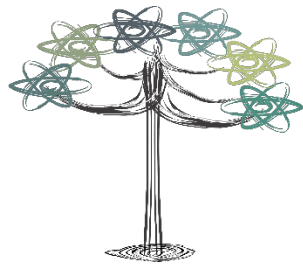
### **Estabilidade, degradação e tempo de vida de filmes finos de PSIF-DBT em diferentes solventes**

Kaike Pacheco<sup>1</sup>, Luana Wouk<sup>2</sup>, Maiara Bassi<sup>3</sup>, Luana Wouk<sup>2</sup>, Lucimara Roman<sup>4</sup>

<sup>1</sup> *Universidade Federal do Paraná, Departamento de Física*

Com a crescente necessidade de geração de eletricidade, estudos têm sido feitos em busca de novas fontes de energia limpa, e dispositivos fotovoltaicos são o principal assunto de várias pesquisas. OPVs (fotovoltaicos orgânicos - como são conhecidos) apresentam vantagens sobre as células solares inorgânicas como baixo peso, produção de baixo custo esperado, mas principalmente sua flexibilidade.

O uso dos OPVs ainda é limitado por causa de seu curto tempo de vida quando não encapsulado, mas sua estabilidade pode ser aumentada devido ao encapsulamento. Neste trabalho, estudou-se a estabilidade e o tempo de vida de filmes de copolímeros de PSIF- DBT produzidos por diferentes processamentos, submetendo-os a condições específicas de iluminância, temperatura e umidade. Os filmes foram degradados dentro de uma câmara que simula condições climáticas específicas, desenvolvida em laboratório, de acordo com os padrões internacionais. Utilizando espectroscopia ótica dos filmes degradados, o trabalho procura entender quais condições levam a uma maior redução da eficiência e acelera sua degradação e a mudança na morfologia desses filmes



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **Effects of neuronal variability on the phase synchronization of neural networks**

*Kalel Luiz Rossi<sup>1</sup>, J. P. Silveira<sup>1</sup>, R.C. Budziski<sup>1</sup>, T.L. Prado<sup>1</sup>, S.R. Lopes<sup>1</sup>*

*<sup>1</sup> Universidade Federal do Paraná (UFPR)*

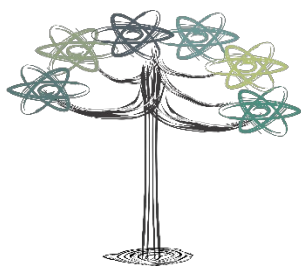
The inter-burst (or inter-spike) interval variability, measured by the standard deviation of the time between bursts (or spikes), is an important neuronal property whose effects on information coding on the brain are widely studied. In the present work, we are interested in the effect the variability has on the phase synchronization of neural networks, which is itself also associated with relevant phenomena, such as memory and information binding.

We calculate the inter-burst interval variability of modified Hodgkin-Huxley neurons, coupled through an Erdos-Renyi connection scheme, and show that it correlates with the degree of phase synchronization of the network, as measured by the Kuramoto order parameter.

We then calculate the number of neurons that are clustered together, as well as the time each neuron stays in the cluster. We find that the variability is inversely proportional to the size and stability of the cluster. If the variability is sufficiently high, neurons stay together only for a few bursts, despite the network as a whole being highly synchronized.

The results thus show that the variability has a strong influence in both the degree of synchronization and the stability of inter-neuron synchronization.





## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### Simulation of Solvent Evaporation to Study the Morphology of an Organic Thin Film\*

Karlisson Rodrigo de A. Sousa<sup>1</sup>, Leandro Benatto<sup>1</sup>, Luana C. W. de Menezes<sup>1,2</sup>,  
Lucimara S. Roman<sup>1</sup>, Marlus Koehler<sup>1</sup>.

<sup>1</sup>*Department of Physics, Federal University of Paraná, Curitiba 81531-990, Paraná, Brazil.*

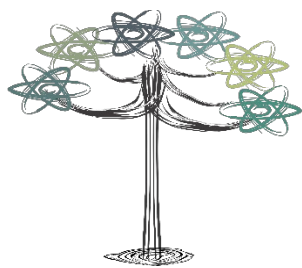
<sup>2</sup>*Center of Innovations – CSEM Brazil, Belo Horizonte 31035-536, Minas Gerais, Brazil.*

The same thin film containing the polymer PTB7-Th, commonly used in organic photovoltaic devices, treated with the halogenated solvent ortho-dichlorobenzene and nonhalogenated solvent ortho-methylanisole demonstrated a difference in their morphology. The cause of the solvent influence on the morphology is not known. In this work, we investigate the origin using computational simulation by molecular dynamics approach and the density functional theory to optimize the material structures to get some equilibrium parameters. We performed simulated solvent evaporation via molecular dynamics, using the method presented by Alessandri *et al.* [1], of two thin films treated with both solvents. It was verified a difference in the energy and morphology, e.g. density and roughness of two films. The results are corroborated with values obtained experimentally by Menezes *et al.* [2].

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\*Work funded by CAPES.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **Photocurrent Generation in Environmentally Friendly Processed Organic Solar Cells: Exploring the Contribution of the Fullerene and Non-Fullerene-Based Molecules**

Leandro Benatto <sup>1</sup>, Maiara de Jesus Bassi <sup>1</sup>, Luana Cristina Wouk de Menezes <sup>1</sup>,  
Lucimara Stolz Roman <sup>1</sup>, Marlus Koehler <sup>1</sup>

<sup>1</sup>*Departamento de Física, Universidade Federal do Paraná (UFPR), Curitiba, PR, Brasil.*

The photocurrent generation in organic solar cells (OSCs) is connected with the charge transfer (CT) dynamics between the electron donor (D) and acceptor (A) materials that compose the active layer [1]. Over the years, the fullerene acceptors (FAs) have stood out for their extremely interesting characteristics, like the spherical geometry and the three low-lying LUMOs (Lowest Unoccupied Molecular Orbitals) [2]. These two main features provide a 3D molecular organization and a high density of unoccupied states that facilitates electron transfer (ET) from the donor and provides high electronic mobility. However, because the FAs have a low light absorption coefficient and high exciton binding energy ( $E_b$ ), their use in OSCs was more related to the dissociation of the excitons generated in the donor materials [3]. With the development of high efficiency non-fullerene acceptors (NFAs), that present high light absorption coefficient and low  $E_b$ , the hole transfer (HT) from acceptor to donor material became an excellent form to increase the photocurrent of OSCs. In addition, low  $E_b$  values allow the decrease of the driving force (defined as the energy difference between the local excited (LE) state and the CT state) ensuring a considerable increase in the open circuit voltage of OSCs [4]. In this work we implement a theoretical study, with Density Functional Theory calculations, of charge transfer dynamics in the D/A interface [5] to explore the main differences between FAs and NFAs for the photocurrent generation in environmentally friendly (with the use of green solvent) processed OSCs.

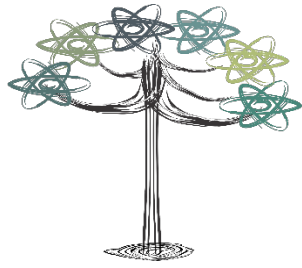
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## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

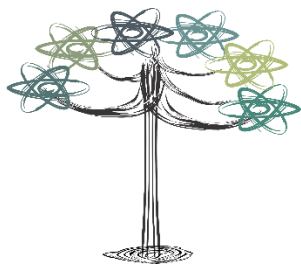
27 e 28 de Junho de 2019

### **Anisotropic MHD equilibria in symmetric systems**

Leonardo C. Souza<sup>1</sup>, Ricardo L. Viana<sup>1</sup>

*<sup>1</sup>Departamento de Física – Universidade Federal do Paraná, Curitiba, Brasil.*

Using a method developed by Clemente, it is possible to obtain anisotropic magnetohydrodynamic equilibrium in axially symmetric systems, from a previously known solution of the Grad-Schluter-Shafranov equation. We generalize this method to symmetric systems described by orthogonal as well as nonorthogonal systems of coordinates. One example is presented in spherical geometries, for which we give an exact analytic solution of the anisotropic MHD equilibrium and analyze the effects of anisotropy in the magnetic field and current density.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **A comparative study on elastic electron scattering from glyoxylic and pyruvic acids**

Leticia S. Maioli and Márcio H. F. Betttega

*Departamento de Física, Universidade Federal do Paraná, 81531-990 Curitiba, Paraná, Brazil*

Glyoxylic acid ( $\text{HCOCOOH}$ , GA), the simplest  $\alpha$ -oxoacid, is constituted by a carboxylic and an aldehyde structural groups. While the pyruvic acid ( $\text{CH}_3\text{COCOOH}$ , PA), the simplest  $\alpha$ -keto acid, differs from the first one by the presence of a methyl group in substitution of one hydrogen atom from the aldehyde unit of glyoxylic acid. Astrochemically, the PA molecule has been detected in carbonaceous meteorites [1] and its study can be motivated by the fact that both systems are suggested to be prebiotic molecules [2]. In the biological view, the dehydrogenated anion form of these composts, namely glyoxylate and pyruvate, are precursors of several key species in metabolic processes [3].

Along this work, we will present the theoretical elastic cross sections for low-energy electron collisions by GA and PA molecules. Our calculations employed the Schwinger multichannel method (SMC) implemented with norm-conserving pseudopotentials (SMCPP) in the static-exchange (SE) and static-exchange plus polarization (SEP) approximations. In addition, both molecules present four conformers that lay in relatively close energy, which are characterized by the relative position of the aldehyde and carboxylic groups. However, we chose to study only the two lowest ones, the Trans-cis (Tc, most stable one) and Trans-trans (Tt) conformers.

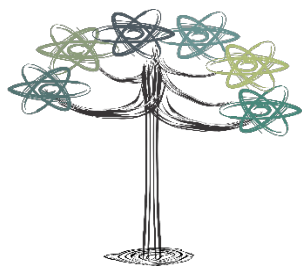
From our cross sections, we could identify the existence of a bound state and two shape resonances, which are respectively assigned as  $\pi^*$  and  $\sigma^*$  anion states. In order to estimate the bound state/resonances energies with the help of an empirical scaling relation, we also performed electronic structure calculations. Consequently, it confirms the presence of a bound anion state and estimates the energy position of the  $\pi^*$  shape resonance in good agreement with our cross section results. Finally, we also present a possibility to associate the resonant states of PA molecule with fragments generated through dissociative electron attachment (DEA) processes reported by Zawadzki *et al.* [4].

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[2] H. D. Ben *et al.*, Orig. Life Evol. Biospheres 36, 39, 2006; E. C. Griffith *et al.*, Orig. Life Evol. Biospheres 43, 341, 2013.

[3] H. L. Kornberg *et al.*, Nature 179, 988, 1957.

[4] M. Zawadzki *et al.*, Phys. Chem. Chem. Phys. 20, 6838, 2018.



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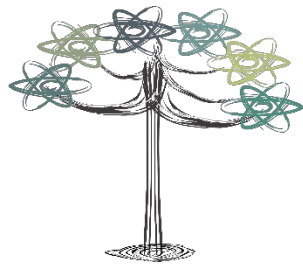
27 e 28 de Junho de 2019

### **Comparison of structural and optical properties of soluble conjugated copolymers with low band-gap for organic solar cells**

Maiara de Jesus Bassi<sup>1</sup>, Leandro Benatto<sup>1</sup>, Luana C. Wouk de Menezes<sup>1</sup>, Camilla Oliveira<sup>1</sup>, Lucimara Stolz Roman<sup>1</sup>

<sup>1</sup> *Universidade Federal do Paraná*

Conjugated copolymers using a donor / acceptor approach (D/A) have shown itself promising in organic solar cells due to improved solar radiation absorption capacity and charge mobility. The copolymers D/A have the alternation of donor and acceptor units of electrons as a characteristic. This feature has been proven to be an effective approach to reduce the gap of the copolymers by internal charge transfer. Within the copolymer class, those having a larger heteroatom that forms the bridge between the conjugate chain and the unconjugated side chain stand out. In particular, the copolymers having silicon atoms to bridge the gap show themselves very promising for the active layer in organic solar cells because of higher crystallinity and better stacking between strands compared to analogous but carbon bridge copolymers. In this study, we investigate the electronic structure, morphological and device performance of films composed by the copolymers PSiF-DBT (Poly[2,7-(9,9-dioctyldibenzosilole)-alt-4,7-bis(thiophen-2-yl)benzo-2,1,3-thiadiazole]) and its analogue without Si, PFO-DBT (Poly[2,7-(9,9-dioctylfluorene)-alt-4,7-bis(thiophen-2-yl)benzo-2,1,3-thiadiazole]) under experimental and theoretical approaches. The results discussed in this study are related to the influence of heavy atom in their physical properties. We have applied the copolymers film as an electron donor in a bilayer structure with a fullerene derivative. We have observed a better photovoltaic performance to the copolymer with Si, resulting in a power conversion efficiency of 2%. Here, we show that our results are capable to provide important insights about the parameters that can be influencing the photovoltaic performance.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

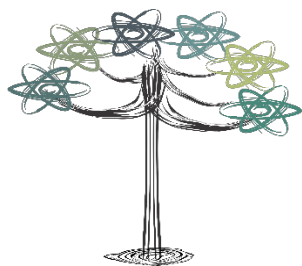
27 e 28 de Junho de 2019

### Ising model and its connections with graph theory

Marcos Gomes<sup>1</sup>, Marco Garcia<sup>2</sup>

<sup>1,2</sup>Universidade Federal do Paraná

There is a connection between partition functions of lattice models (Ising model, Potts model) in statistical physics with graph theory (spanning trees). We are studying those connections to gain some insight on how to understand better the structure of the solution of the Ising model in 2D for all the periodic lattices. Spanning trees are related to the 2D Ising model by means of a Spanning tree generating function  $T(z)$  (STGF). We are also trying to find similar relations in other dimensions, the spanning tree generating function (STGF) satisfies a differential equation involving the probability generating function (also called lattice Green function (LGF)) and gives the spanning tree constant when evaluated at  $z=1$ . We present a new result that provides an integral representation of this function  $T(z)$  for all the periodic lattices. With this result we now are trying to prove a general theorem that relates  $T(z)$  with the Ising model solution for all the periodic lattices.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### Evaluation and Characterization of Electrodes Based on Graphene Oxide and PEDOT:PSS

Matheus Felipe Fagundes das Neves<sup>1</sup>, Bruno Gabriel Alves Leite Borges<sup>2</sup>, Soheila Holakoei<sup>2</sup>, Carolina Ferreira de Matos<sup>3</sup>, Aldo José Gorgatti Zarbin<sup>4</sup>, Maria Luiza Miranda Rocco<sup>2</sup> and Lucimara Stolz Roman<sup>1</sup>

<sup>1</sup>*Universidade Federal do Paraná (Departamento de Física),*

<sup>2</sup>*Universidade Federal do Rio de Janeiro (Instituto de Química),*

<sup>3</sup>*Universidade Federal do Pampa (Departamento de Química),*

<sup>4</sup>*Universidade Federal do Paraná (Departamento de Química)*

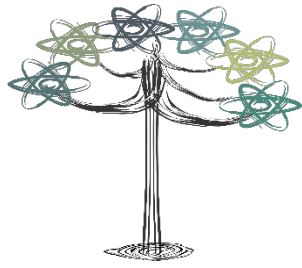
During the last few years, organic photovoltaics have become a very important technology for energy saving. They present advantages as low-cost fabrication by easy processing routes using nontoxic materials deposited on flexible substrates, opening to a wide range of applications. In this scope, the present study attempts to investigate thin films with different mass ratio of graphene oxide with PEDOT:PSS (1, 5, 10 and 100 % v/v), as a new electrode approach. We compare structural differences on the morphology of the films and investigate the ordering and orientation of the molecular films by surface and bulk-sensitive X-ray Absorption Spectroscopy. We have evaluated the ultrafast electron dynamics (in femtosecond range) employing the resonant Auger spectroscopy. We additionally measured the sheet resistance as a function of transmittance and torsion cycle. In order to improve the conductivity we performed a simply treatment with ethylene glycol by drop and dip casting and evaluated the morphology, electrical and optical properties. The materials become more conductive and transparent. The treatment also standardized the film. Moreover, different deposition techniques were evaluated, as spin coating and airbrush. This study shows that GO:PEDOT:PSS has potential to substitute ITO as flexible electrode in photovoltaic devices.

#### Acknowledgements:

The authors are grateful to CAPES, CNPq and LNLS – Brazil. This work has been partially supported by the 'Companhia Paranaense de Energia – COPEL' research and technological development program, through the PD 2866-0470/2017 project, regulated by ANEEL.

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[1] B. Borges, S. Holakoei, M. das Neves, L. de Menezes, C. Matos, A. Zarbin, L. Roman, M. Rocco, Molecular orientation and femtosecond charge transfer dynamics in transparent and conductive electrodes based on graphene oxide and PEDOT:PSS composites, Phys. Chem. Chem. Phys., 2019, 21, 736-743.



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27 e 28 de Junho de 2019

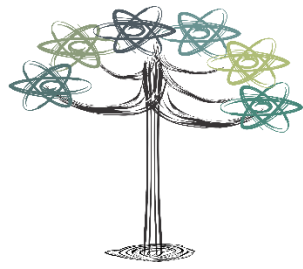
### **Changes in the wave function at avoided crossings**

Matheus Rolim Sales<sup>1</sup>, Fabio Marcel Zanetti<sup>1</sup>

<sup>1</sup> *Departamento de Física, Universidade Federal do Paraná, Curitiba, Paraná 81531-990, Brazil*

Avoided crossings are common in the energy spectra of classically chaotic quantum systems. They are displayed in diagrams where the energy levels are plotted versus a varying parameter. In this work we examine the wave functions of the desymmetrized Sinai billiard to show that when two (or three) energy levels undergo an avoided crossing, the morphology of their wave functions is swapped. We also show that successive avoided crossings along a fictive curve, giving rise to solitonlike structures, are intimately related to how strongly a system is scarred and to the persistence of the bouncing-ball states.





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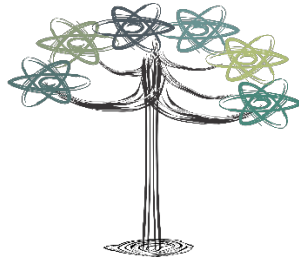
27 e 28 de Junho de 2019

### Quantum Reference Frames and the Invariance of Information

Matheus F. Savi<sup>1</sup> e Renato. M. Angelo<sup>1</sup>.

<sup>1</sup> *Department of Physics, Federal University of Paraná, Curitiba, Brazil.*

Einstein's relativity and Schrödinger's quantum mechanics define the age of modern physics. The former has taught us that space and time are transmutable quantities: a spacelike event for one observer may be a timelike event for another, meaning that they might disagree when comparing individual measurements of length and time intervals concerning the same event. Nonetheless, there is a quantity in which all (inertial) observers will agree upon, i.e., invariant under a transformation of reference frames, called the interval; a quantity wherein time and space stand on equal footing. In quantum mechanics, however, a similar result has not been put forward. Namely, is there an invariant quantity under the transformation of quantum reference frames? If so, can it be decomposed into transmutable quantities? Here we show that, through a protocol of local unrevealed projective measurements, the information about a system plays this role if, and only if, we consider the Observer-Observed Symmetry, in which we allow the reference frame, observer, to be regarded as an interacting physical system and, thus, to be observed. The OO Symmetry is mandatory if one wishes to preserve the invariance of information.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **Stickiness Effect on Oseledets Splitting Statistic in Mixed Phase Space Hamiltonian Flows**

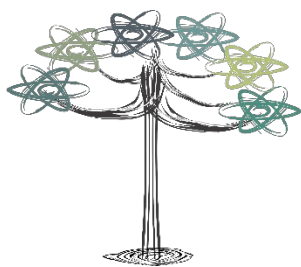
Miguel Angel Prado Reynoso<sup>1</sup>, Marcus Werner Beims<sup>2</sup>.

<sup>1,2</sup> *Universidade Federal do Paraná*

Stickiness is a temporary confinement of orbits in a particular region of the phase space before they diffuse to a large region, for example, around of island of stability, which is surrounding by cantori with small holes.

Considering a classical chaotic dynamical system and invertible, the Oseledets Splitting are invariant subspaces associated with the Lyapunov Spectrum, allowing to investigate the directions of expansion and contractions of the given system in each point of the phase space. The Covariant Lyapunov vectors (CLV) are defined which unitary vectors spanning the Oseledets splitting. The CLV give information about the tangencies between invariant manifolds of the system, providing a measure of the degree of partial-hyperbolicity. Such tangencies were shown to be relate with the sticky motion for a Hamiltonian map.

In this work we analyse the possibility to relate the statistic of this invariant subspace (tangencies, expansions and contractions ) with the effect of stickiness in Hamiltonian flows with mixed phase space.



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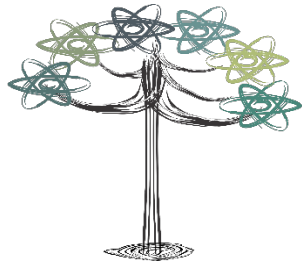
27 e 28 de Junho de 2019

### **Electron scattering by Formamide and N-dimethylformamide molecules.**

Murilo de Oliveira Silva<sup>1</sup>, Márcio Henrique Franco Bettega<sup>2</sup>.

<sup>1,2</sup> *Federal University of Paraná*

In recent years studies of electron collisions by molecules have grown. Such growth is due to the many applications found in daily life, some of them on the industrial and biological fields. In the industry, the collision process occurs in the constitution of cold plasmas, in which they are used for the manufacture of microelectronic devices. These are responsible for modifying the surface's properties and materials, also used in materials removal or cleaning. As in biology, radiation is known to cause damage to our tissue, which is also caused by low-energy electrons. Researchers have shown that low-energy electrons are responsible for breaking DNA strands, where those breaks are caused by the imprisonment of temporary electrons. So, in this work, we study the electron scattering by the molecule of Formamide ( $\text{HCONH}_2$ ). We have also studied the effect of methylation on the Formamide molecule, that is, we added methyl ( $\text{NH}_3$ ) to the molecule, resulting in N-dimethylformamide ( $\text{HCONH}(\text{CH}_3)_2$ ). We employed the Schwinger multichannel (SMC) method with pseudopotentials (SMCPP) in the static-exchange (SE) and static-exchange plus polarization (SEP) approximations. We present calculations of the cross sections for the molecules mentioned above. Thus, we investigated the resonance peaks in the calculations, where it was also possible to estimate the position of the resonance by the Koopmans' Theorem through a electronic structure calculation. With the estimated resonance, we obtained for the Formamide the resonance at approximately 2.08 eV, for the N-dimethylformamide the estimated resonance was at 2.06 eV. According to the calculations performed, the SEP level is in good agreement with the value estimated by Theorema de Kooppmans'



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **Perpendicular magnetization switching induced by spin-orbit torques in Pt/(Co/Ni) multilayers**

Nicholas Figueiredo Prestes<sup>1,3</sup>; Sophie Collin<sup>1</sup>; Juliana Zarpellon<sup>3</sup>; Laurent Vila<sup>2</sup>;  
Nicolas Reyren<sup>1</sup>; Dante Homero Mosca<sup>3</sup>; Jean-Marie George<sup>1</sup>.

<sup>1</sup> *Unité Mixte de Physique CNRS, Thales, Univ. Paris-Sud, Université Paris-Saclay, 91767  
Palaiseau, France.*

<sup>2</sup> *Université Grenoble Alpes, CEA, CNRS, INP-G, INAC, F-38054 Grenoble, France.*

<sup>3</sup> *Universidade Federal do Paraná, Programa de Pós-Graduação em Física, Curitiba, Brasil.*

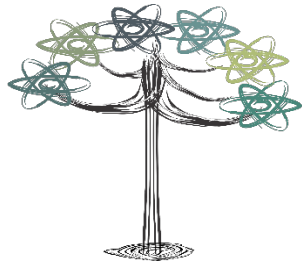
The discovery of reliable and efficient methods to manipulate the magnetization of nanostructures is an important objective of current spintronics research. In the last decades, predictions by Slonczewski and Berger helped the development of the spin valves, devices where the magnetic reversal is thoroughly explained by the spin-transfer torque (STT) effect. The principle was successfully incorporated in MRAM devices for writing operation. Nevertheless, it is still required to lower the current for magnetic reversal.

An alternative approach takes advantage of the spin-dependent scattering observed in heavy metals and other materials to generate the spin currents. Because different mechanisms (spin Hall effect [1], Rashba effect and Edelstein effect in 2D materials) concomitantly contribute to torques on ferromagnetic layer, we speak more generally of spin-orbit torques (SOT). SOT has the advantage to eliminate the need for a polarizing magnetic layer and to dissociate the spin current from the charge current. When enough moment (large SOT) is transferred to the ferromagnetic material, the associated torque may reverse the magnetization, which also depends of the external field and the charge current direction [2].

We present experimental results of an ongoing work on the perpendicular magnetization reversal induced by SOT of micronic and submicronic patterned [Co(0.2 nm)/Ni(0.6 nm)]x3 multilayered films on top of a 6-nm-thick Pt electrode. Reversal was probed using Anomalous Hall effect measurements and Kerr microscopy was used to reveal details of the switching process. We also present phase diagrams of the switching conditions for an angular distribution of the in-plane field. In light of these experiments, we discuss the ingredients needed to understand our results: the damping and field-like torques, and the DMI.

#### References:

- [1] J. Sinova ,et al. Rev. Mod. Phys. 87, 1213 (2015).
- [2] J.-C. Rojas-Sánchez, et al. Appl. Phys. Lett. 108, 082406 (2016)..



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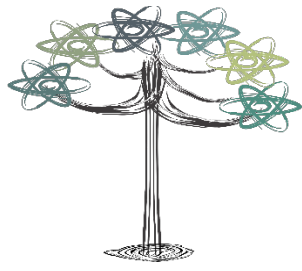
27 e 28 de Junho de 2019

### **Steering and irreality in pure states**

Paulo Muraro Ferreira<sup>1</sup>, Renato Moreira Angelo<sup>1</sup>

<sup>1</sup> *Universidade Federal do Paraná, Departamento de Física, Curitiba, Paraná*

Steering is a quantum resource related to the possibility of using two entangled subsystems A and B, along with classical communication, to collapse the B subsystem to different substates conditioned to distinct choices of measurements in the A subsystem. Equivalently, the joint probability of a steerable state can be written as the convex sum of separable probabilities, where one of the marginal probabilities is compatible with the quantum theory and the other is a generic probability distribution. There are two main criteria for detection of steering for continuous variables: the first is set up on the violation of the uncertainty principle for observables of the B subsystem inferred based on observables measured on the A subsystem, and the second is centered on entropic functions. Even though entanglement guarantees steering for any pure state, both aforementioned criteria fail to identify such non-local aspect for some entangled pure states. The goal of this work is to investigate a realistic description for one of the subsystems of pure bipartite states, and, as a result, to regain the notion of steering, and also to develop a measure of steering, based on realism and constructed upon expected values, that is more effective than the known criteria for continuous variables. In order to do so, we consider elements of reality associated to the canonical pair  $(q,p)$  and implemented by projectors built upon bosonic coherent states. Applying the realism based criteria for the study of several entangled states, we see that our criteria always reveals steering when the state is not separable, even when the existing criteria do not.



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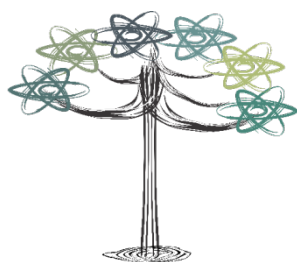
27 e 28 de Junho de 2019

### **Synchronization and intermittency in a network of networks based on human brain**

R. C. Budzinski<sup>1</sup>, B. R. R. Boaretto<sup>1</sup>, T. L. Prado<sup>1</sup>, S. R. Lopes<sup>1</sup>

<sup>1</sup> *Departamento de Física, Universidade Federal do Paraná, Curitiba, Brazil*

Synchronization of coupled systems has been explored since the last century and find application in different areas where the connection architecture plays an important role. In this scenario, mathematical and computational approaches have been used in the context of the complex network in order to investigate many problems related to the neural systems. In fact, the synchronization is very important to the neural networks and it is related to the functioning of the brain, since neurological disorders may be related to the lack or excess of synchronization. The dynamical properties of phase synchronization and intermittent behavior of neural systems can be studied using a network of networks structure based on an experimentally obtained human connectome for healthy and Alzheimer-affected brains. It is considered a network composed of 78 neural subareas (subnetworks) coupled with a mean-field potential scheme. Each subnetwork is characterized by a small-world topology, composed of 250 bursting neurons simulated through the Rulkov map. Using the Kuramoto order parameter, it is possible to demonstrate that healthy and Alzheimer-affected brains display distinct phase synchronization and intermittency properties as a function of internal and external coupling strengths. In general, for the healthy case, each subnetwork develops a substantial level of internal synchronization before a global-stable-phase-synchronized state has been established. For the unhealthy case, despite the similar internal subnetwork synchronization levels, it is identified higher levels of global phase synchronization occurring even for relatively small internal and external coupling. Using recurrence quantification analysis, namely the determinism of the network mean-field potential, it is observed regions where the healthy and unhealthy networks depict nonstationary behavior, but the results denounce the presence of a larger region of intermittent dynamics for the case of Alzheimer-affected networks. At last, a possible theoretical explanation based on two locally stable but globally unstable states is discussed in the context of the network of networks.



# I WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

21 a 23 de Março de 2018

## **Growth and characterization of Mn-Ge thin films on GaAs substrates**

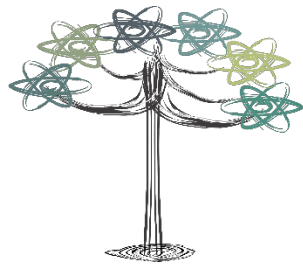
R. C. de Oliveira<sup>1</sup>, D. H. Mosca<sup>1</sup>, J. Varalda<sup>1</sup>

<sup>1</sup>Universidade Federal do Paraná

Thin films of  $\text{Mn}_{100-x}\text{Ge}_x$  ( $43 \leq x \leq 71$ ) were grown on GaAs (111) and GaAs (001) using the molecular beam epitaxy technique. The deposits were carried out for 1 hour with the substrate in a temperature of 200 ° C. X-ray photoelectron spectroscopy and reflection high-energy electron diffraction was done in situ. Stoichiometry of the samples was obtained through the analysis of photoelectron spectroscopy, which was also used to demonstrate that the desorption process of the oxides of the substrates was successful. The results of the reflection high-energy electron diffraction reveal typical patterns of a film with a smooth surface, except in the case of the sample  $\text{Mn}_{29}\text{Ge}_{71}$  that presented a pattern with continuous lines (indicating a smooth surface) together with dots (indicating a rough surface). This peculiar pattern was attributed to a possible surface structure formed by nanostructures of  $\text{Mn}_5\text{Ge}_3$ ,  $\text{Mn}_{11}\text{Ge}_8$ , and Ge. In the case of the other samples, no significant change in the electron diffraction patterns was observed as a function of stoichiometry. The results of X-ray diffraction indicate that all the samples show the same phases ( $\text{Mn}_5\text{Ge}_3$ ,  $\text{Mn}_{11}\text{Ge}_8$ , and Ge) independent of the stoichiometry or orientation of the substrate. The results presented in this study indicate the possibility of the existence of self-assembled nano-columns of  $\text{Mn}_5\text{Ge}_3$  with the c axis oriented parallel to the normal of the surface of the films.

### Acknowledgments:

The authors thank LORXI (Laboratório de Óptica de Raios X e Instrumentação) from Universidade Federal do Paraná, and CNPq by financial support. One of us (R. C. O.) thanks CAPES (Coordenação de Aperfeiçoamento de Pessoal de Nível Superior) scholarship.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **Correlated Brownian motion and diffusion of defects in spatially extended chaotic systems**

Sidney T. da Silva<sup>1</sup>, Ricardo. L. Viana<sup>2</sup>

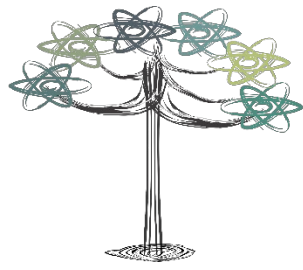
<sup>1</sup> *Federal University of Paraná.*

<sup>2</sup> *Federal University of Paraná*

3

One of the spatiotemporal patterns exhibited by coupled map lattices with nearest-neighbor coupling is the appearance of chaotic defects, which are spatially localized regions of chaotic motion with a particle-like behavior. Chaotic defects display random behavior and diffuse along the lattice with a Gaussian behavior. In this note we investigate some dynamical properties of chaotic defects in a lattice of coupled chaotic quadratic maps. Using a recurrence-based diagnostic we found that the motion of chaotic defects is well-represented by a stochastic time series with a power-law spectrum, i.e. a correlated Brownian motion. The correlation exponent corresponds to a memory effect in the Brownian motion, and increases with a system parameter as the diffusion coefficient of chaotic defects.





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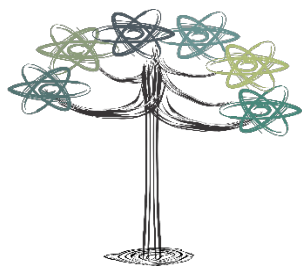
27 e 28 de Junho de 2019

### Quantum Work: A Mechanical Perspective

Thales Augusto Barbosa Pinto Silva<sup>1</sup>, Renato Moreira Angelo<sup>2</sup>.

<sup>1,2</sup> *Universidade Federal do Paraná.*

Work can be regarded as one of the most fundamental concepts of Thermodynamics. Within the quantum framework, it received in the 1970's a well grounded definition which has been successfully applied to contexts involving classical external driving mechanisms. However, many deep foundational questions have not been satisfactorily addressed up until now. For instance, it is not clear (i) how to define work for a few-particles autonomous system involving both spatial and spin degrees of freedom, (ii) how to define heat, and distinguish it from work, within a fundamental quantum-mechanical perspective, (iii) how to extend these concepts to scenarios involving many particles, (iv) what are the roles played by information discard and realism in the emergence of equilibrium thermodynamics, irreversibility, and for the validation of fluctuation theorems. Here we discuss some routes to assess these problems departing from classically oriented models.



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27 e 28 de Junho de 2019

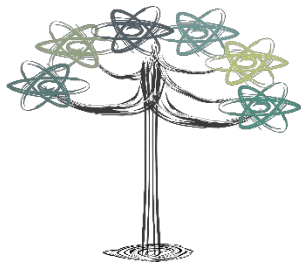
### **X-ray spectroscopy and extended cluster model calculations of $\text{MoO}_2$ , $\text{RuO}_2$ , and $\text{Rh}_2\text{O}_3$**

V. Stoeberl<sup>1</sup>, E. B. Guedes<sup>1</sup>, M. Abbate<sup>1</sup>, R. J. O. Mossaneck<sup>1</sup>, F. Abud<sup>2</sup>, R. F. Jardim<sup>2</sup>.

<sup>1</sup> *Departamento de Física, Universidade Federal do Paraná*

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In the present report, we investigate the structure of three different 4d transition metal oxides (TMO's): a distorted  $d^2$  metal ( $\text{MoO}_2$ ), a regular  $d^4$  metal ( $\text{RuO}_2$ ), and a regular  $d^6$  insulator ( $\text{Rh}_2\text{O}_3$ ). The main goal of this work is to study different experimental techniques - in particular, Cooper Minimum Method and Resonant Photoemission - applying them in the description of the electronic structure of the compounds. Both techniques are useful to separate partial contributions of oxygen and metal states for each valence band region of the spectra. These two results are compared and discussed concerning the pros and cons in each case. In order to reproduce and interpret the experimental spectra, we use the extended cluster model, 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 of all compounds in comparison with its ionic values. This can be attributed to the strong mixing between MT 4d - O 2p that is present in all cases. The predominance of an 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  $\text{MoO}_2$ . Ru 3p and Rh 3p results show the main peak and some satellite structures which are both screened by oxygen. Coherent screening is also present in the  $\text{RuO}_2$  satellites. The  $\text{MoO}_2$  and  $\text{RuO}_2$  VB XPS results show coherent screening at the Fermi level, confirming their metallic behavior. A combination of Davis and Feldkamp's theory for interaction between discrete and continuous states and our extended cluster model which considers electronic correlation, intra-atomic exchange, and metal-ligands hybridization, brought unprecedented results about resonant photoemission of 4d TMO's, reproducing signals and relative intensities of the resonance curves with an excellent agreement. All the presented experimental spectra were reproduced using the same set of parameters.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### **Macroscopic properties of rarefied gases considering quantum effects in Interatomic collisions of He**

Yonathan Daviran and Felix Sharipov

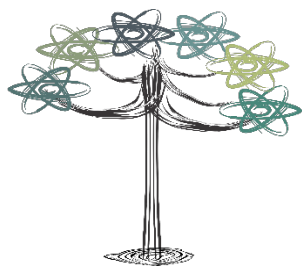
*Departamento de Física, Universidade Federal do Paraná, Curitiba, Brazil*

In the present work, the quantum dispersion effects for helium are implemented, using direct simulation Monte Carlo (DSMC) [1] method, macroscopic properties for helium gas are obtained using the kinetic theory [2] and compared with situation when the quantum effects are neglected. The classical problems such as Couette and Fourier flows[2] are solved with and without quantum effects of interatomic collisions[3]. The method was used to study the influence of the interatomic potential in rarefied gases, considering the intermolecular interaction that is justified at high temperatures for heavy gases. However, the quantum effects in intermolecular interactions is not negligible for light gases and should be noted that the influence of quantum effect can be larger for flows with a larger temperature variation.

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## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### Positron collisions with targets of biological and technological relevance

Alessandra Souza Barbosa

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Curitiba, Paraná, Brazil*

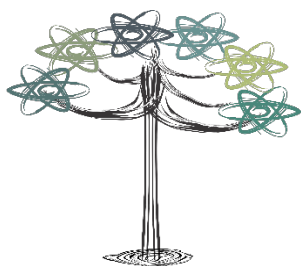
Positron physics attracts great interest due to its fundamental, technological and biological applications. And since many of its applications are based on basic interactions of positrons with molecules, positron-scattering studies become a cornerstone towards understanding the underlying physics of these interactions. In recent years, thanks to the advent of better theoretical methodologies and computers to perform the simulations, theoretical positron-molecules studies have gained new breath. At the same time, experimental advances have considerably improved the data available in the literature.

However, positron scattering calculations can be a difficult task due some intrinsic problems. For example, besides the inelastic process already observed in electron-scattering, the incoming positron can capture one of the electrons of the target to form positronium (Ps). Moreover, Ps formations can be responsible for a large amount of the total cross section for positron impact energies over the positronium formation threshold. Even more troublesome, at energies below the Ps formation and electronic excitation thresholds, the agreement between the theoretical calculations and experimental data is far from good. This is mainly due to a poor description of the polarization potential for positron scattering.

In recent years, our group has put a lot of effort in order to provide some reliable results for positron scattering by molecules and systems of technological and biological relevance. For example, employing the Schwinger multichannel method [1], we have performed extensive studies in order to improve the description of the polarization potential for two small non-polar molecules, allene and silane [2,3]. It is worth mentioning that the fact that for the first time a bound state was predicted by an *ab initio* scattering calculation [2]. Our group has also been leading the efforts of the description of positron interactions with biological systems, such as the pyrimidine [4] and tetrahydrofuran molecules.

In this talk we will discuss some of our recent theoretical results on positron scattering by molecules of technological and/or biological relevance. Some of the target molecules include benzene and its azaderivatives, pyridine and pyrimidine, tetrahydrofuran and a discussion of how the description of the polarization effects can be improved in scattering calculations.

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## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

### Nanopartículas em Física Médica

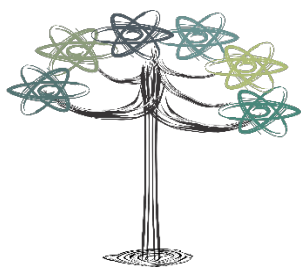
Oswaldo Baffa

*Departamento de Física, FFCLRP-Universidade de São Paulo, Ribeirão Preto, Brasil.*

Nanopartículas (NPs) de metais nobres, como ouro e prata, são potencialmente biocompatíveis e apresentam propriedades plasmônicas capazes de intensificar a interação com a luz visível. Devido ao alto número atômico, essas NPs metálicas também aumentam a probabilidade de interação com a radiação ionizante, especialmente na faixa de energia onde o efeito fotoelétrico é predominante, possibilitando diferentes aplicações médicas como o reforço da dose depositada em dosímetros ou tumores que contenham NPs metálicas [1]. Devido às propriedades plasmônicas, elas podem ainda aumentar a sensibilidade de dosímetros de radiação aferidos por métodos luminescentes por meio da luminescência acoplada aos plásmons [2]. Além das NPs metálicas, NPs magnéticas também encontram ampla aplicação na área médica podendo ser utilizadas em separação magnética, agentes de contraste em imagens de ressonância magnética, marcação de células, hipertermia e marcadores magnéticos. A biosusceptometria AC tem sido utilizada para estudos da dinâmica dessas NPs magnéticas [3,4]. Outra possibilidade é o estudo da relaxação de Néel em NPs que estão ligadas a células e com isso determinar a quantidade de células [5]. Esses estudos exigem tanto o desenvolvimento de novas rotas síntese de NPs, a produção de amostras e experimentação animal, além de instrumentação adequada para as medidas, oferecendo uma excelente possibilidade de treinamento associada à geração de novos conhecimentos. Nesse trabalho, serão reportados os resultados relacionados ao uso de NPs metálicas e magnéticas em Física Médica.

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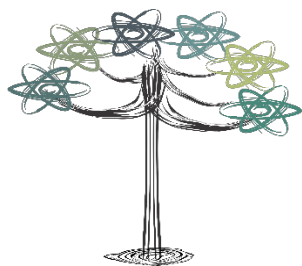
27 e 28 de Junho de 2019

### **A Física de Sabores no Large Hadron Collider: Matéria vs. Antimatéria, partículas exóticas e anomalias**

*Carla Göbel Burlamaqui de Mello.*

*Departamento de Física, PUC-Rio.*

Como é sabido, o Modelo Padrão descreve as interações (forte, eletromagnética e fraca) entre as partículas fundamentais — 6 quarks e 6 léptons — que se distribuem em três famílias de sabores. A chamada Física de Sabores no setor dos quarks representa um ambiente extremamente rico para o estudo de uma série de fenômenos, tais como a Violação de Carga-Paridade (e sua conexão com a assimetria matéria-antimatéria no Universo), oscilações partícula-antipartícula, formação de estados exóticos como tetraquarks e pentaquarks, entre outros. A Física de Sabores também abre uma importante janela para a busca de Nova Física (além do Modelo Padrão) através do estudo de decaimentos raros e proibidos, que poderiam ser significativamente afetados pela presença de novas partículas ou interações. Nesta palestra, serão apresentadas as motivações e uma visão geral do programa de Física de Sabores do LHC, com ênfase aos resultados mais recentes e importantes do experimento LHCb.



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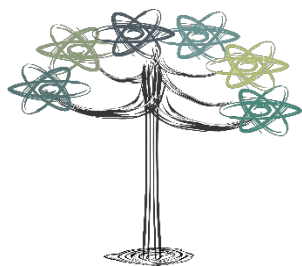
### **Materials Design through reactive molecular dynamics techniques**

Cristiano F. Woellner<sup>1</sup>

<sup>1</sup> *Departamento de Física, Universidade Federal do Paraná*

In this talk I will show how reactive molecular dynamics (MD) techniques have been used to design materials in a variety of different applications. These techniques make feasible to simulate systems of millions of atoms but with the novelty of allowing chemical reactions (creating/breaking chemical bonds) at the same time. To highlight this versatility, I will describe in more detail one of our recently published works. This work refers to a new class of 3D porous carbon-based structures called Schwarzites. They are 3D porous solids with periodic minimal surfaces having negative Gaussian curvatures and can possess unusual mechanical, thermal and electronic properties. I will present a comparative study about the mechanical behavior of some Schwarzite structures at nano length scale using MD simulations and 3D printed versions at centimeter length scales based on molecular models. The results suggest that these 3D printed structures hold great promise as high load bearing and impact-resistant materials due to a unique layered deformation mechanism that emerges in these architectures during loading. Therefore, easily scalable techniques such as 3D printing can be used for exploring mechanical behavior of various predicted complex geometrical shapes to build innovative engineered materials with tunable properties.





## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

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### **Armazenamento e Processamento de Dados: Passado, Presente, Futuro**

Daniel Lottis

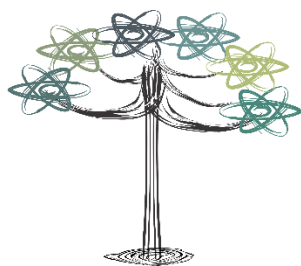
*IEEE Magnetics Society, Santa Clara Valley Chapter*

e

*CLSE Consulting*

A função de computadores como ferramenta de trabalho na Física tem uma história rica e fascinante. Também é verdade que conhecimentos de Física têm sido de importância central para o avanço da computação. Nesta palestra a abordagem da vasta temática descrita no título terá um enfoque principal definido pela experiência do palestrante como Físico na área de magnetismo aplicado. As origens da gravação magnética em mídias como arame magnético, discos rígidos, discos flexíveis, e fita serão brevemente recapitulados. O mesmo ocorrerá com memória magnética RAM ou MRAM, partindo do armazenamento em "bits" consistindo de anéis de material magnético, passando pelos primeiros chips MRAM integrados onde multicamadas substituíram os anéis. Os avanços na densidade de armazenamento de informação, rapidez de acesso, e custo serão citados, bem como os avanços tecnológicos que permitiram estas melhorias, e sua dependência nos correspondentes avanços em nosso conhecimento de Física. Para tanto, faremos referência a conceitos como gravação longitudinal e perpendicular; mídias granulares e em filmes finos; leitura indutiva e magnetoresistiva; coercividade magnética da mídia; gravação assistida energeticamente (EAMR, HAMR, MAMR); e mídia com bits discretos ou "Bit Patterned Media". Em seguida, será apresentada a nova disciplina denominada "Spintrônica", na qual tanto a carga quanto o spin dos elétrons são aproveitados para controlar fenômenos e dispositivos magnéticos. A revisão de tecnologias já estabelecidas será completada com discussões da junção de tunelamento magnético (MTJ, ou "magnetic tunneling junction") que serve tanto como sensor para leitura em HDDs quanto dispositivo de memória em circuitos integrados MRAM. Tecnologias de ponta, que são candidatos para inclusão em produtos a ser comercializados durante a próxima década, serão discutidos brevemente, com ênfase em estruturas que aproveitam o chamado "Spin-Orbit Torque" (SOT). Este torque, relacionado com o efeito Spin-Hall, é utilizado para realizar ou ao menos ajudar na inversão de "bits". A apresentação fará referência aos gigantescos centros de dados coletivamente descritos como "Cloud"; à profunda transformação na maneira em que HDs são empregados como componentes em tais datacenters; e ao conceito de hierarquia de armazenamento de dados. Tecnologias de memória do tipo "storage-class" (armazenamento) como PCM e Memristors serão também brevemente discutidos. A abordagem de processamento de dados incluirá conceitos como o uso de elementos como os MTJs empregados como unidades simulando atividade neurológica; elementos de lógica fazendo uso de Spintrônica; como os conceitos de "in-memory computing" e "near memory computing"; e os avanços de tecnologias abertas como a arquitetura RISC-V. A palestra incluirá um período de perguntas e respostas antes do encerramento.





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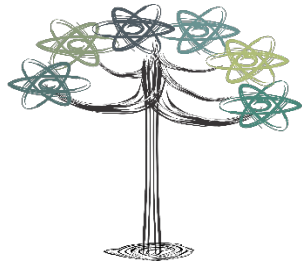
### **Processos ópticos não lineares induzidos por pulsos de femtossegundos**

Emerson C. Barbano<sup>1</sup>, Sérgio C. Zilio<sup>2</sup>, Lino Misoguti<sup>2</sup>.

<sup>1</sup> *Departamento de Física, Universidade Federal do Paraná, CP 19044, 81531-980, Curitiba, PR, Brasil.*

<sup>2</sup> *Instituto de Física de São Carlos, Universidade de São Paulo, CP 369, 13560-970, São Carlos, SP, Brasil.*

Ao longo da história do estudo de fenômenos ópticos, na maior parte do tempo acreditou-se que todo meio óptico fosse linear, ou seja, sua resposta, descrita pela polarização induzida no meio devido à interação da radiação com a matéria, seria linearmente proporcional ao campo elétrico da luz. Porém, em uma época relativamente recente e, principalmente, após o advento do laser em 1960, passou-se a estudar a interação luz-matéria no regime de altas intensidades, o que tornou possível observar respostas não lineares do meio com relação à amplitude do campo incidente. Assim, pode-se dizer que a óptica não linear é o ramo da óptica que descreve as propriedades de um material durante sua interação com uma luz intensa. Em laboratório, esta radiação é normalmente obtida com o uso de lasers de pulsos ultracurtos, como os de femtossegundos, por exemplo. Desde então uma grande variedade de fenômenos ópticos não lineares passaram a ser descobertos e modelados, ocasionando uma revolução tecnológica com aplicações no setor industrial, na área da saúde e em pesquisas científicas diversas. Nesta apresentação farei uma breve introdução à óptica não linear e discutirei a determinação do índice de refração não linear, que é um parâmetro extremamente relevante no desenvolvimento de dispositivos puramente fotônicos. Mostrarei estudos relacionados à sua determinação que fazem uso de uma técnica moderna baseada no efeito de rotação da polarização elíptica. Esta técnica possibilita uma determinação precisa do índice de refração não linear da amostra sob investigação e pode ser empregada na caracterização de sólidos, líquidos e gases, dentre outras aplicações.



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### **Teoria H: Uma Descrição Unificada para Fenômenos de Flutuação – de Turbulência a Lasers Aleatórios “and Beyond”**

Giovani L. Vasconcelos<sup>1</sup>

<sup>1</sup>*Departamento de Física, UFPR, Curitiba, PR.*

Neste seminário apresentarei uma teoria unificada desenvolvida no nosso grupo para descrever fenômenos de flutuação em sistemas complexos que possuem várias escalas de tempo e comprimento [1-4]. Turbulência é um exemplo prototípico dessa classe de sistemas. Nesse caso, a energia injetada no fluido gera grandes estruturas coerentes (turbilhões) que se partem em turbilhões menores, os quais dão origem a turbilhões ainda menores, etc, gerando assim uma "cascata de energia", até que a energia é dissipada por forças viscosas na escala microscópica. O fluxo de energia ao longo dessa cascata acontece de forma intermitente, levando a flutuações aleatórias na diferença de velocidade do fluido entre sucessivos intervalos de tempo e posições. Essa dinâmica estocástica multiescala invariavelmente leva a distribuições não Gaussianas que exibem assimetria e caudas pesadas. Fenômenos de flutuação com uma dinâmica hierárquica semelhante ocorrem em vários outros sistemas da física e de áreas interdisciplinares, como a economia e biologia. Nossa teoria propõe uma abordagem geral na qual as distribuições de equilíbrio em sistemas hierárquicos são obtidas como uma mistura ponderada de distribuições Gaussianas de equilíbrio local. A distribuição peso é obtida a partir de um modelo estocástico hierárquico de intermitência que admite uma solução exata em termos da função G de Meijer ou de uma nova função especial que introduzimos, a chamada função R [4] que generaliza as funções G. A distribuição resultante é obtida analiticamente em termos dessas funções, o que nos permite calcular explicitamente as caudas das distribuições. A teoria possui também uma abordagem equivalente através de um princípio da máxima entropia [3]. Serão apresentadas aplicações recentes da teoria H para vários sistemas, tais como turbulência em fluidos [1,4], lasers aleatórios [2], flutuações de preços no mercado financeiro [1] e dinâmica de busca de alimentos em ecologia [5]. Perspectivas de desenvolvimento da teoria H para sistemas quânticos e relativísticos serão brevemente discutidas.

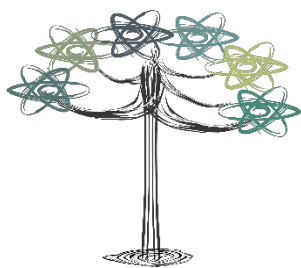
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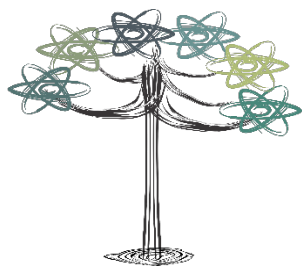
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### **Sirius: a nova fonte de luz síncrotron brasileira**

Harry Westfahl Jr.

*Leboratório Nacional de Luz Síncrotron, Campinas*

O Laboratório Nacional de Luz Síncrotron (LNLS) está construindo o Sirius, a maior e mais complexa infraestrutura científica já construída no país e uma das primeiras fontes de luz síncrotron de quarta geração do mundo. O Sirius colocará o país entre as lideranças mundiais neste tipo de tecnologia e permitirá analisar materiais sintéticos e biológicos em escalas de tempo e comprimento sem precedentes no estado da arte atual, alavancando o desenvolvimento de pesquisas em áreas estratégicas como energia, alimentos, meio ambiente, saúde, defesa e muitas outras. Neste seminário serão introduzidos aspectos fundamentais da ciência com luz síncrotron, as principais características do Sirius e de suas primeiras estações experimentais e o status atual do projeto.



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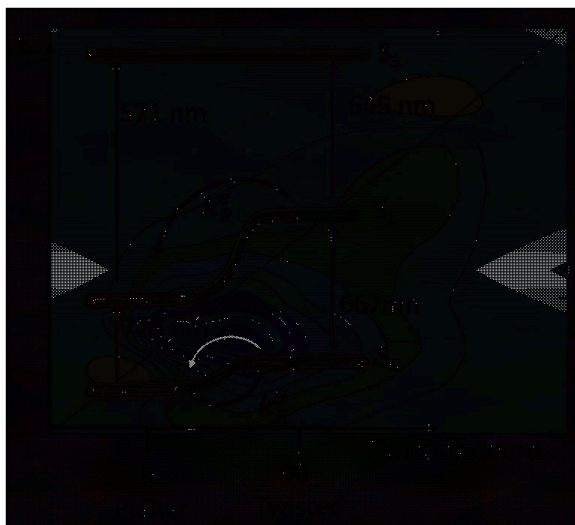
### **Fundamentals and Applications of Multidimensional Ultrafast Spectroscopy**

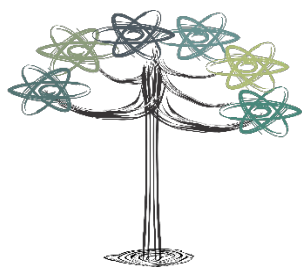
Ismael A. Heisler

*Departamento de Física, Universidade Federal do Paraná*

In this talk I will provide an overview of our efforts at understanding fundamental molecular properties. I will discuss cutting edge methods and relate to our most recent efforts in establishing a new 2D electronic spectroscopy (2D- ES) laboratory. This is a versatile spectroscopic method that can provide detailed information about a variety of inter- and intramolecular dynamics in excited states.

We aim to apply 2D ES to study energy and charge transfer in multichromophoric porphyrin arrays that are being synthesized with the specific purpose of mimicking the ability of natural light-harvesting pigment-protein complexes to collect photon energy and transmit it efficiently to reaction centres. A thorough understanding of the ground and excited-state dynamics, including structural motions, will be critical for their use in technological applications. In this talk I will focus on the structural dynamics and coherences of porphyrin-based structures. In the ground state, due to a low twisting energy barrier, the dimer presents a distribution of twisted conformations ranging from planar to fully twisted. Excitation to the first singlet excited state however drives the system to a mainly planar conformation. This is captured in the rising cross peak in the evolving 2D spectra. This result is interpreted with a model, which incorporates information obtained by fluorescence, transient absorption and computational results. Furthermore, I will present our results regarding electronic and vibrational coherences and discuss how to interpret them and how they can be used to clarify some of the previously published results on light-harvesting complexes.





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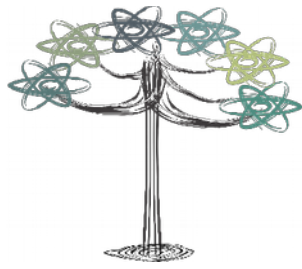
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### **Homenagem ao Professor Ivo Alexandre Hümmelgen**

Marlus Kohler, José Pedro Mansueto Serbena.

*Departamento de Física, Universidade Federal do Paraná.*

Nesse colóquio iremos homenagear a memória do Prof. Ivo A. Hümmelgen, falecido em Março último. Iremos ressaltar alguns importantes fatos da carreira e da vida acadêmica do Prof. Ivo, que deu contribuições extremamente relevantes para a consolidação da pós-graduação do DFIS. O Prof. Ivo era um físico experimental destacado, tendo sido um dos pioneiros no estudo da eletrônica orgânica no Brasil. Foi o fundador dessa linha de pesquisa no DFIS e ajudou a formar muitos professores que hoje compõe os quadros de nosso departamento, além de pesquisadores que atuam em diversas universidades brasileiras e no exterior. Acima de tudo, o Prof. Ivo foi também uma grande figura humana, que inspirou a vida de seus estudantes, colegas e amigos.



## II WORKSHOP DO PROGRAMA DE PÓS- GRADUAÇÃO EM FÍSICA

27 e 28 de Junho de 2019

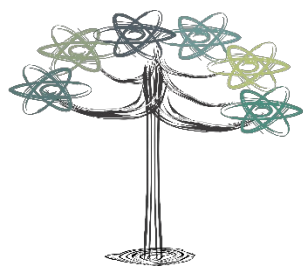
### **Transições em redes complexas neuronais analisadas por microestados de recorrências**

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O estudo de redes complexas neuronais é de amplo interesse devido a seu potencial relativo a possibilidades científicas e tecnológicas. Dentre os diversos comportamentos dinâmicos de interesse presentes em redes complexas neuronais, abordaremos o fenômeno de sincronização e a forma como ela ocorre para rede de neurônios não idênticos. No presente trabalho serão apresentadas novas possibilidades de aplicações dos microestados de recorrências, em particular, o cálculo da entropia de Shannon dos mesmos para o estudo de redes complexas neuronais. Os microestados de recorrências são extrações de matrizes  $\mathbf{N} \times \mathbf{N}$  dos gráficos de recorrência (**RP**), os quais são matrizes binárias, onde 1 (0) representa estados da trajetória dinâmica recorrentes (não-recorrentes) a outros estados da trajetória dinâmica relativo a um raio de tolerância. A construção ou perda de padrão devido a sincronização ou dessincronização da rede, altera de forma substancial a informação presente na rede, tornando a entropia bastante adequada a essas caracterizações. Por fim, apresentaremos relações entre a diversidade neuronal e como essa altera a estrutura das transições entre estado sincronizado e dessincronizado.



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### **Breve histórico do Programa de Pós-Graduação em Física da Universidade Federal do Paraná**

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O Programa de Pós-Graduação em Física do Setor de Ciências Exatas da Universidade Federal do Paraná foi criado em 1983, inicialmente a nível de Mestrado, tendo sido ampliado em 1994 com a criação do Doutorado. Foi o primeiro curso de pós-graduação em Física *stricto sensu* no estado do Paraná e um dos primeiros na região Sul do Brasil. Neste seminário pretendemos mostrar, de forma breve, o histórico do Programa, enfatizando a contribuição de docentes e discentes na construção e na manutenção do curso, atualmente um dos mais importantes do país.