Scientific report 2015

Pesquisa em Dark Matter
Astroparticle Physics

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ICTP-SAIFR - São Paulo - Brazil

Processo: 2013/01792-8

Período: 01/10/2013 - 30/12/2015
Scientific report 2015

Nicolás Bernal
ICTP-SAIFR - São Paulo - Brazil
Processo: 2013/01792-8

I joined the ICTP-SAIFR two years ago; my contract started on October 1st 2013. The present report details my activities in 2015.

1 Research

We propose and study a scalar extension of the Standard Model which respects a $\mathbb{Z}_3$ symmetry remnant of the spontaneous breaking of a global $U(1)_{DM}$ symmetry. Consequently, this model has a natural dark matter candidate and a Goldstone boson in the physical spectrum. In addition, the Higgs boson properties are changed with respect to the Standard Model due to the mixing with a new particle. We explore regions in the parameter space taking into account bounds from the measured Higgs properties, dark matter direct detection as well as measurements of the effective number of neutrino species before recombination. The dark matter relic density is determined by three classes of processes: the usual self-annihilation, semi-annihilation and purely dark matter $3 \rightarrow 2$ processes. The latter has been subject of recent interest leading to the so-called ‘Strongly Interacting Massive Particle’ (SIMP) scenario. We show under which conditions our model can lead to a concrete realization of such scenario and study the possibility that the dark matter self-interactions could address the small scale structure problems. In particular, we find that in order for the SIMP scenario to work, the dark matter mass must be in the range 7-115 MeV, with the global symmetry energy breaking scale in the TeV range.

In the context of Self-Interacting Dark Matter as a solution for the small-scale structure problems, we consider the possibility that Dark Matter could have been produced without being in thermal equilibrium with the Standard Model bath. We discuss one by one the following various dark matter production regimes of this kind: freeze-in, reannihilation and dark freeze-out. We exemplify how these mechanisms work in the context of the particularly simple Hidden Vector Dark Matter model. In contrast to scenarios where there is thermal equilibrium with the Standard Model bath, we find two regimes which can easily satisfy all the laboratory and cosmological constraints. These are dark freeze-out with $3 \rightarrow 2$ annihilations and freeze-in via a light mediator. In the first regime, different temperatures in the visible and the Dark Matter sectors allow us to avoid the constraints coming from cosmic structure formation as well as the use of non-perturbative couplings to reproduce the observed relic density. For the second regime, different couplings are responsible for Dark Matter relic density and self-interactions, permitting to surpass BBN, X-ray, CMB and direct detection constraints.

Dark matter with strong self-interactions provides a compelling solution to several small-scale structure puzzles. Under the assumption that the coupling between dark matter and the Standard Model particles is suppressed, such strongly interacting massive particles (SIMPs) allow for a successful thermal freeze-out through $N \rightarrow n$ processes, where $N$ dark matter particles annihilate to $n$ of them. In the most common scenarios, where dark matter stability
is guaranteed by a $\mathbb{Z}_2$ symmetry, the seemingly leading annihilating channel, i.e. $3 \to 2$ process, is forbidden, so the $4 \to 2$ one dominate the production of the dark matter relic density. Moreover, cosmological observations require that the dark matter sector is colder than the thermal bath of Standard Model particles, a condition that can be dynamically generated via a small portal between dark matter and Standard Model particles, à la freeze-in. This scenario is exemplified in the context of the Singlet Scalar dark matter model.

2 Publications

   Nicola S Bernal (ICTP - SAIFR), Xiaoyong Chu (ICTP)
   arXiv:1510.08527 [hep-ph], submitted to JCAP.

   Nicola S Bernal (ICTP - SAIFR), Xiaoyong Chu (ICTP), Camilo Garcia-Cely (Brussels U.), Thomas Hambye (Brussels U.), Bryan Zaldivar (LAPTh)
   arXiv:1510.08063 [hep-ph], submitted to JCAP.

   Nicola S Bernal (ICTP - SAIFR), Camilo Garcia-Cely (Brussels U.), Rogério Rosenfeld (ICTP - SAIFR)

3 Proceedings

1. WIMP and SIMP Dark Matter from the Spontaneous Breaking of a Global Group.
   Nicola S Bernal (ICTP - SAIFR), Camilo Garcia-Cely (Brussels U.), Rogério Rosenfeld (ICTP - SAIFR)
   Nuclear Physics B Proceedings Supplement, in press.

   Nicola S Bernal (ICTP - SAIFR), Jaime E. Forero-Romero (U. de los Andes), Raghveer Garani (Bonn U.), Sergio Palomares-Ruiz (Valencia, IFIC)
   Nuclear Physics B Proceedings Supplement, in press.

4 Seminars, Conferences & Workshops

4.1 Seminars

I have been invited to present my work in different institutions:

4.2 Conferences and Workshops

I participated in international conferences and workshops where I had the opportunity to present my research.

   ‘$Z_2$ SIMP Dark Matter’. ICTP - SAIFR. São Paulo, Brazil.

   ‘The SIMPlest Dark Matter Model’. ICTP - SAIFR. São Paulo, Brazil.

   ‘From Self- to Strongly-Interacting DM’. Caxambu, Brazil.

   ‘SIMPs → SIMPs’. ICTP. Trieste, Italy.

15. May 28 to Jun. 1, 2015. Beyond WIMPs: From Theory to Detection


   ‘SIMP Dark Matter’. ICTP - SAIFR. São Paulo, Brazil.
4.3 Other Meetings

18. Aug. 20-21, 2015. 1st Brazilian CTA Collaboration Meeting
   IAG - USP. São Paulo. Brazil.

   ICTP - SAIFR. São Paulo. Brazil.

5 Organization of Seminars

I have been actively organizing seminars in the ICTP-SAIFR.

5.1 Astrophysics & Cosmology Journal Club (AC/JC)

In November 2013, I created and organized, together with Saeed Mirshekari, a journal club devoted to cosmology and astrophysics: The Astrophysics & Cosmology Journal Club (AC/JC). It has been scheduled every two weeks on Mondays 11:00 am in the room #1 of the ICTP-SAIFR. I remained involved in the organization until August 2015.

5.2 Latin American Webinars on Physics

Working in the ICTP-SAIFR, the South American Center for Fundamental Research, I set up and organized a series of Webinars on high energy physics focused on the integration of the Latin American community that is running since February 2015. The webinars are scheduled every second Wednesday at 1500 GMT via the Google+ Channel and offline on the YouTube Channel. This effort is done in collaboration with other physicists scattered around the globe: Jorge S. Diaz (KIT, Germany), Germán A. Gómez-Vargas (PUC-Chile & INFN), Joel Jones-Perez (PUCP, Peru), Roberto A. Lineros (IFIC-U.Valencia/CSIC, Spain), Diego Restrepo (U. Antioquia, Colombia), Avelino Vicente (U. Liège, Belgium), Federico Von der Pahlen (U. Antioquia, Colombia) and Fabio A. Pereira dos Santos (PUC-Rio de Janeiro, Brazil). Audience and speakers have been returning an excellent feedback. As of today, 15 webinars took place and the series will continue next year.

6 Reviewer for international journals

This year I refereed articles in the following international journals:

- Journal of Cosmology and Astroparticle Physics (JCAP)
- Journal of Physics G: Nuclear and Particle Physics

7 Joint supervision

I co-supervised with Prof. Rogério Rosenfeld a Master student, working on the solution of the Boltzmann equations for SIMP dark matter.

- Master student Luan Vinícius Koerich
  IFT - UNESP, São Paulo, Brazil
8 Research plans for 2016

Next year I will continue my research on Physics Beyond the Standard Model, focusing on various aspects of the phenomenology of the Dark Matter. I will for instance keep studying the impact of potential deviations of the sphericity of the dark matter halo profile, and the potential gamma-ray indirect detection consequences. Another project is the study of the eventual connection between the dark matter and the standard model and the possibility that these two sectors share an asymmetry. This asymmetry could be the responsible for the dark matter relic abundance measured today and the baryon asymmetry of the Universe. A third area of work will be the self-interacting dark matter produced by the recently proposed SIMP paradigm, that interacts with the standard model via a kinetic mixing portal.

Triaxiality of Dark Matter Halos
Nicolás Bernal (ICTP-SAIFR), Lina Necib (MIT) and Tracy R. Slatyer (MIT).
Although commonly assumed to be spherical, dark matter halos are predicted to be non-spherical by N-body simulations and their asphericity has a potential impact on the systematic uncertainties in dark matter searches. The evaluation of these uncertainties is the main aim of this work, where we will study the impact of aspherical dark matter density distributions in Milky-Way-like halos on direct and indirect searches. We will look into the sphericity of the dark matter halos in dark matter-only simulations versus dark matter and baryon simulations of Illustris. We will also analyze the implications of the sphericity of dark matter in indirect detection signals in general and the galactic center gamma-ray excess in particular.

Sharing the Asymmetry between the Dark and the Visible Sectors
Nicolás Bernal (ICTP-SAIFR), Chee Sheng Fong (IF-USP) and Nayara Fonseca (DESY).
We will study a dark matter scenario where the visible sector and the dark sector share a common asymmetry. The two sectors are connected through heavy mediators with baryon or lepton number, allowing the standard model baryon asymmetry to be shared with the dark matter via annihilation processes. The present-day abundance of dark matter is then set by thermal freeze-out of this annihilation process, yielding an asymmetric version of the WIMP miracle as well as promising signals for indirect detection experiments.

Self-Interacting Dark Matter through the Kinetic Mixing Portal
Nicolás Bernal (ICTP-SAIFR) and Josef Pradler (Vienna, ÖAW).
It is expected that the Dark Matter communicates with the Standard Model via the exchange of a mediator. There are different portals in the SM, one of them corresponding to the kinetic mixing of a new $U(1)_D$ symmetry. This vector portal is of particular interest as it leads to bilinear mixing with the photon and is thus experimentally testable, and at the same time allows for a vector which is naturally light.
Scientific report 2014

Nicolás Bernal
ICTP-SAIFR - São Paulo - Brazil

I joined the ICTP-SAIFR last year; my contract started on October 1st 2013.

• Conferences, Workshops & Seminars
This year I have attended and presented my work in different international scientific events. On one hand, I presented my work about the ‘Systematic uncertainties from halo asphericity in dark matter (DM) searches’ in several international conferences: X Simposio Latinoamericano de Física de Altas Energías SILAFAE (December 23-28) in Medellín - Colombia, XXXV Encontro Nacional de Física de Partículas e Campos (September 15-19) in Caxambu - Brazil, Astroparticle Physics 2014 (June 23-28) in Amsterdam - Netherlands, PLANCK 2014 (May 26-30) in París - France and Mini Workshop on Cosmology (February 20-21) at the ICTP - SAIFR in São Paulo - Brazil.
On the other hand, I have also been invited to present my research on ‘$Z_3$ DM and Goldstone bosons’ and visit different research institutes like: Departamento de Raios Cósmicos e Cronologia, Universidade Estadual de Campinas (September 2) in Campinas - Brazil, Physikalisches Institut of the Universität Bonn (July 18) in Bonn - Germany and the Centro de Física Teórica de Partículas, Instituto Superior Técnico (June 3) in Lisboa - Portugal.
In addition I also played an active role in the local journal clubs taking place in São Paulo. On September 25th in the Joint USP/UNESP Journal Club I presented an article about the ‘Baryon asymmetry of the universe from DM annihilations’, on March 10th in the Astrophysics & Cosmology Journal Club (AC$^κ$JC) I discussed the paper ‘Discovering DM with gamma-rays from the galactic center’ and on March 6th I talked about ‘SIMP DM’ in the Particle Physics Journal Club.

• Astrophysics & Cosmology Journal Club (AC$^κ$JC)
Together with Saeed Mirshekari we organize a journal club devoted to subjects related to cosmology and astrophysics. It has been scheduled every two weeks on Mondays 11:00 am in the room #1 of the ICTP-SAIFR. We had national and international invited speakers like: Rita Bernabei (Università e INFN Roma Tor Vergata), Loïc Le Tiran (IAG - USP), Manuela Vecchi (USP - São Carlos), Ernany Schmitz (IFT - UNESP), Enrique Gaztañaga (Instituto de Ciencias del Espacio - Barcelona), Raul Abramo (IF - USP), Eduardo Pontón (ICTP - SAIFR), Riccardo Sturani (IFT - UNESP), Leandro Beraldo (IF - USP), Saeed Mirshekari (ICTP - SAIFR), Irène Balmès (IF - USP), Fabien Lacasa (ICTP - SAIFR), Nicolás Bernal (ICTP - SAIFR) and Morgan Le Delliou (IFT - UNESP). The (AC$^κ$JC) has been well received and has been attended by people from both the UNESP (ICTP + IFT) and the USP (IAG + IF). It will continue during the next semester.

• Publication
In collaboration with Jaime E. Forero-Romero (Andes U., Bogotá), Raghunveer Garani (Bonn U.) and Sergio Palomares-Ruiz (Valencia U., IFIC), I wrote and article that got accepted in JCAP: JCAP 1409 (2014) 004. The title is: ‘Systematic uncertainties from...
halo asphericity in DM searches’. Abstract: Although commonly assumed to be spherical, DM halos are predicted to be non-spherical by N-body simulations and their asphericity has a potential impact on the systematic uncertainties in DM searches. The evaluation of these uncertainties is the main aim of this work, where we study the impact of aspherical DM density distributions in Milky-Way-like halos on direct and indirect searches. Using data from the large N-body cosmological simulation Bolshoi, we perform a statistical analysis and quantify the systematic uncertainties on the determination of local DM density and the so-called $J$ factors for DM annihilations and decays from the galactic center. We find that, due to our ignorance about the extent of the non-sphericity of the Milky Way DM halo, systematic uncertainties can be as large as 35%, within the 95% most probable region, for a spherically averaged value for the local density of 0.3-0.4 GeV/cm$^3$. Similarly, systematic uncertainties on the $J$ factors evaluated around the galactic center can be as large as 10% and 15%, within the 95% most probable region, for DM annihilations and decays, respectively.

- Research plans for the year 2015
  Currently with Camilo García-Cely (Université Libre de Bruxelles, Belgium) and Rogério Rosenfeld (IFT - UNESP) we are studying the phenomenology of a model of scalar DM with a global $U(1)$ symmetry that spontaneously breaks into a $Z_3$. This scenario has a very rich phenomenology that contains for example the possibility of explaining the extra relativistic degrees of freedom (dark radiation) that could be in the Planck data, and the possibility of solving some problems at small scales in the ΛCDM model like the ‘missing satellites’, the ‘core versus cusp’ and the ‘too big to fail’. On top of that, in this model the generation of the DM relic abundance can happen via different mechanisms, namely self-annihilation, semi-annihilation and the very recently proposed $3 \rightarrow 2$ annihilation: ‘$Z_3$ DM from a global $U(1)$ breaking, dark radiation and the SIMP scenario’.

  Additionally with Camilo García-Cely and Thomas Hambye (Université Libre de Bruxelles, Belgium) we are studying the generation of the DM relic density in the Hidden Vector DM model. DM could be made of massive gauge bosons whose stability doesn’t require to impose by hand any discrete or global symmetry. Stability of gauge bosons can be guaranteed by the custodial symmetry associated to the gauge symmetry and particle content of the model. The hidden sector interacts with the Standard Model particles through the Higgs portal quartic scalar interaction in such a way that the gauge bosons behave as thermal WIMPs. This can lead easily to the observed DM relic density in agreement with the other various constraints. We are examining regions of the parameter space that were previously excluded by the DM abundance but that are now reopened via new DM generation mechanisms.

  A third project that has to be finished during 2015 is with Tracy Slatyer (MIT, USA). We are looking for the asymmetries in the possible triaxiality of the Milky Way DM halo. We are comparing the quadrant-based asymmetry for our various DM halo profiles with the astrophysical backgrounds and the maps of the gamma-ray emission from the diffuse model and the point sources measured by the Fermi satellite.

  In recent years, a possible connection between the abundances of baryons and DM has been explored. Even if so far most of the studies have been in the context of the so-called asymmetric DM, a very different mechanism, dubbed ‘WIMPy baryogenesis’, has been recently proposed to relate the baryon asymmetry to (symmetric) DM annihilation. In
both cases the DM candidate is a usual WIMP, thermally produced, with mass and interactions at the weak scale. However, there are alternate mechanisms of DM genesis involving Feebly Interacting Massive Particles (FIMPs), interacting so feeble with the thermal bath that they never attain thermal equilibrium. With some collaborators we already have studied realizations of the WIMPy baryogenesis and we are pursuing the research now focusing in the possibilities of generating simultaneously the observed baryon asymmetry of the universe and the measured FIMP DM relic abundance.
I joined the ICTP-SAIFR a couple of months ago; my contract started on October 1st 2013.

- **Journal Club on Particle Phenomenology**
  On November 14th I led a discussion in the Journal Club on particle phenomenology about a recent paper on ‘Dark matter production from Goldstone boson interactions and implications for direct searches and dark radiation’.

- **Astrophysics & Cosmology Journal Club (AC$^\varpi$JC)**
  Together with Saeed Mirshekari we started a Journal Club devoted to subjects related to cosmology and astrophysics. It has been scheduled for every two weeks on Mondays 11:00 am in the room #3 of the ICTP-SAIFR. Each AC$^\varpi$JC session has two parts: First, we have a free discussion on a few recent papers suggested by the audience; then we focus on a paper that is presented in more details. Prof. Rogério Rosenfeld (IFT-UNESP), Dr. Arman Esmaili Taklimi (Unicamp) and Prof. Gary Steigman (Ohio State University) have discussed papers in the AC$^\varpi$JC. The Journal Club has been well received and has been attended by people from both the UNESP (ICTP + IFT) and the USP (IAG + IF). It will continue in the next semester.

- **Publication**
  Just after joining the ICTP-SAIFR, an article that I wrote in collaboration with Stefano Colluci (Uni Bonn, Germany), François-Xavier Josse-Michaux (CFTP, Portugal), Juan Racker (IFIC, Spain) and Lorenzo Ubaldi (Uni Bonn, Germany) got accepted for publication in JCAP: *JCAP 1310 (2013) 035*. The title is: ‘On baryogenesis from dark matter annihilation’. In that paper we study in detail the conditions to generate the baryon asymmetry of the universe from the annihilation of dark matter (DM). This scenario requires a low energy mechanism for thermal baryogenesis, hence we first discuss some of these mechanisms together with the specific constraints due to the connection with the DM sector. Then we show that, contrary to what stated in previous studies, it is possible to generate the cosmological asymmetry without adding a light sterile dark sector, both in models with violation and with conservation of $B - L$. In addition, one of the models we propose yields some connection to neutrino masses.
**Research plans for the year 2014**

Currently with Raghuveer Garani (Uni Bonn, Germany), Jaime Forero-Romero (Uni Andes, Colombia) and Sergio Palomares-Ruiz (IFIC, Spain) we are studying the systematic uncertainties induced by halo triaxiality in WIMP DM searches. In order to quantify the interaction rates in direct and indirect detection experiments, one has to have under control not only the particle physics properties of the DM particle (mass, cross sections and annihilation/decay channels) but also the astrophysical properties. In particular one has to know the local DM relic density $\rho_0$ for direct detection and the whole shape of the DM halo for indirect detection. Let me note that what enters in the flux for indirect detection is a $J$ factor that corresponds to the integral of the DM halo profile along the line of sight. The most promising method to learn about the functional forms of the density profiles is through sophisticated N-body simulations of structure formation in the universe. Important halo properties such as DM density radial profile, halo mass concentration and halo shapes can be discerned from this technique. In general, N-body simulations predict that the DM mass distribution in the halo to be aspherical and favor triaxial shapes. The impact of the triaxial of the halo on local observables such as the DM local density, the velocity dispersion and the $J$ factors can be significantly large and induces systematic uncertainties. Using the DM-only Bolshoi simulation we are discussing the impact of halo triaxiality in the determination of DM event rates. We are noticing that there can be large deviations of $\rho_0$ and $J$ factor from that of the spherically averaged values for triaxial halos. These deviations can be very large for $\rho_0$ and about 20% for $J$, for typical triaxial halos.

In recent years, a possible connection between the abundances of baryons and DM has been explored. Even if so far most of the studies have been in the context of the so-called asymmetric DM, a very different mechanism, dubbed ‘WIMPy baryogenesis’, has been recently proposed to relate the baryon asymmetry to (symmetric) DM annihilation. In both cases the DM candidate is a usual WIMP, thermally produced, with mass and interactions at the weak scale. However, there are alternate mechanisms of DM genesis involving Feebly Interacting Massive Particles (FIMPs), interacting so feeble with the thermal bath that they never attain thermal equilibrium. With some collaborators we already have studied realizations of the WIMPy baryogenesis and we are pursuing the research now focusing in the possibilities of generating simultaneously the observed baryon asymmetry of the universe and the measured FIMP DM relic abundance.

I also plan to start collaborations with the local people (UNESP and USP), in particular with Prof. Rogério Rosenfeld, Prof. Eduardo Pontón and Prof. Gary Steigman.
1. $\mathbb{Z}_2$ SIMP Dark Matter.
   Nicolás Bernal (ICTP - SAIFR), Xiayong Chu (ICTP)
   arXiv:1510.08527 [hep-ph], submitted to JCAP.

   Nicolás Bernal (ICTP - SAIFR), Xiayong Chu (ICTP), Camilo Garcia-Cely (Brussels U.),
   Thomas Hambye (Brussels U.), Bryan Zaldivar (LAPTh)
   arXiv:1510.08063 [hep-ph], submitted to JCAP.

   Nicolás Bernal (ICTP - SAIFR), Camilo Garcia-Cely (Brussels U.), Rogério Rosenfeld
   (ICTP - SAIFR)

   Nicolás Bernal (ICTP - SAIFR), Jaime E. Forero-Romero (U. de los Andes), Raghuveer Garani (Bonn U.),
   Sergio Palomares-Ruiz (Valencia, IFIC)
5. **On Baryogenesis from Dark Matter Annihilation.**

Nicolás Bernal (ICTP - SAIFR), Stefano Colucci (Bonn U.), François-Xavier Josse-Michaëux (Lisbon, CFTP & Lisbon, IST), Juan Racker (Valencia, IFIC), Lorenzo Ubaldi (Bonn U.)


6. **WIMP and SIMP Dark Matter from the Spontaneous Breaking of a Global Group.**

Nicolás Bernal (ICTP - SAIFR), Camilo Garcia-Cely (Brussels U.), Rogério Rosenfeld (ICTP - SAIFR)


7. **Systematic Uncertainties from Halo Asphericity in Dark Matter Searches.**

Nicolás Bernal (ICTP - SAIFR), Jaime E. Forero-Romero (U. de los Andes), Raghuveer Garani (Bonn U.), Sergio Palomares-Ruiz (Valencia, IFIC)

Electronic properties and quantum transport in non-periodic systems

Dr. José Hugo Garcia Aguilar

supervised by
Prof. Dr. Nathan Berkovits

December 3, 2015
Introduction

One of the milestone of solid state physics is the possibility to consider a solid as a periodic arrangement of atoms, this allows to represent the Hamiltonian of the system in the momentum-space, where one can use different analytic and computational methods to obtain the spectral properties. However, there are systems intrinsically aperiodic such as quasicrystals, amorphous solids, atomic clusters and highly disordered systems, where the momentum-space approach is usually inadequate.

One way to describe these non-periodic system is to use real-space tight-binding models where each atom in the solid is described as a set of localized states that overlap with others in a given neighborhood. Therefore, the number of atoms is what limits this approach for practical situations and in general cannot be cannot be much larger than $10^4$.

In the last year I and coworker developed an efficient numerical method based on Chebyshev polynomials to calculate spectral quantities of real-space tight-binding Hamiltonian with over $10^7$ sites[1], this approach can be greatly benefited by the use of parallel environment and we used graphics processing units (GPU) to this purpose which allow us to obtain speed-ups of up to 100 times compare with a single core CPU. During my time at ICTP-SAFIR the focus of my research is to further develop this method and to apply it to different types of non-periodic systems.

1 Research during the period August-December 2015

1.1 Electronic properties of graphene with T-site adatoms

Graphene is a carbon allotrope where the atoms are organized in a two-dimensional honeycomb lattice and its electrons behave as relativistic massless Dirac Fermions near the Fermi energy as shown in Fig.1. This two features made of graphene a promising material for the future electronics and an interesting playground for fundamental research[2, 3, 4].

![Graphene lattice and dispersion relation](image.png)

Figure 1: (a) The primitive lattice vector and the nearest neighbors of the honeycomb lattice. (b) The dispersion relation of the Honeycomb lattice. Inset: The dispersion near the Fermi energy
The graphene’s lattice can be nicely describe by a tight-binding Hamiltonian of the form:

\[ H_g = \sum_{\langle i,j \rangle} a^\dagger(R_i)b(R_j) + h.c \]  

(1.1)

where \( \langle i,j \rangle \) represents a summation over the nearest neighbors shown in Fig.1.a, \( a^\dagger[b] \) and \( a[b] \) represents the creation and destructions operator for an electron in the sublattice \( a[b] \) of the lattice.

By considering a modified version of this model, Kane and Mele showed that one can use graphene as a template for a topological insulator \([5]\), provided that the honeycomb structures posses an strong spin-orbit coupling (SOC). One of the most remarkable properties of topological insulator is the presence of a robust spin-polarized current without the need of any external magnetic field, which make them a promissory type of systems for spintronics. Therefore it is desirable to use the massless Dirac electrons of graphene as the carriers of this spin polarized current. Unfortunately, spin-orbit coupling in pristine graphene is too weak (\( \sim 1 \mu eV \)) but Balakrishnan et al. showed in their work that a large SOC can be achieve by deposition of a small concentration of hydrogen on graphene \([6]\). The physics behind this enhancement is still not clearly understood, but some insights can be gained from the calculations of Gmitra et al\([7]\), where they present a tight-binding model based on a Anderson one impurity model

\[ H = H_g + \varepsilon_h \sum_m h_{m\sigma}^\dagger h_{m\sigma} + T \sum_{\langle m,i \rangle} h_{m\sigma}^\dagger c_{i\sigma} + h.c + H_{SOC} \]  

(1.2)

where \( \varepsilon_h \) is the energy of the localized level at the hydrogen atom, \( T \) is the hybridization potential between hydrogen and graphene and \( H_{SOC} \) represents a local spin-orbit interaction generated by the adsorption of hydrogen into graphene, which has the following form

\[ H_{so} = \frac{2i}{3} \sum_{\langle i,j \rangle} c_{i\sigma}^\dagger c_{j\sigma'} [\Lambda_{BR}(\hat{s} \times \hat{d}_{ij})_z]_{\sigma\sigma'} + \frac{i}{3} \sum_{\langle\langle i,j \rangle \rangle} c_{i\sigma}^\dagger c_{j\sigma'} \left[ \frac{\Lambda_{c}^c}{\sqrt{3}} \nu_{ij} \hat{s}_z + 2 \Lambda_{PIA}^c (\hat{s} \times \hat{D}_{ij})_z \right]_{\sigma\sigma'} \]  

(1.3)

\[ \Lambda_{BR}, \Lambda_{PIA} \]

a representation of the neighborhood for each term is given in Fig.2.b. To find the values of the tight-binding parameters Gmitra et al. fit their model with the electronic band structure obtained by density functional theory. We developed a methodology to fit electronic band structure using

![Figure 2: (Color online) (a) First-principles calculations of electric dipole moments induced by hydrogen adatoms on a 5 x 5 supercell. Directions of the dipole moments are shown by arrows; the sphere radii correspond to the dipole magnitudes. (b) Hopping scheme of the tight-binding model showing the relevant orbital and spin-orbit coupling parameters. [7] (a) (b)](image)
We reproduce implement a methodology to reproduce the results of Gmitra et. al by combining density functional theory (DFT) with genetic algorithm (GA) in order to find the tight-binding parameters of the model, we were able to reproduce the results of Gmitra et. al and found the parameters of a better fit. We also present explore the possibility of absorbing OH intro graphene instead of H as the possible source of Spin-Orbit coupling.

1.2 Electronic properties of two-dimensional quasicrystals

Another important non-periodic system are quasicrystals, where the atoms organized themselves into a highly-ordered structure which is entirely aperiodic such as the one shown in Fig.4. One way to model quasicrystals is to construct a crystalline approximant, which is a large atomic arrangement whose behavior in a crystalline structure is similar to one of a quasicrystal[8]. However, when
these approximants are small, they are more metallic than quasicrystals and doesn’t accurately reproduce many features related to the lack of periodicity such as criticality, and fractality of the wave function[8].

Figure 5: (a) $\sigma_{xy}$ (dashed line) and $\sigma_{xx}$ (solid line) calculated using the method by Garcia et. all, for two different temperatures $k_B T = 0$ (black) and $k_B T/t = 0.004$ (red). (b) Electronic density of states (c) $\sigma_{xx}$ away from the Dirac point where Shubnikov-de Haas oscillations can be observed for $k_B T/t = 0.002$ (black) , $k_B T/t = 0.004$ (red), $k_B T/t = 0.008$ (blue) for $N = 2 \times 128 \times 1024$ sites and $t=2.8$eV.

In this project, we are using the Kernel polynomial method in order to study approximants with more than $10^5$ sites, and we explore the criticality of these using a local distribution approach[9, 10]. In this approach one look at the distribution of local quantities such as de local density of states(LDOS) to obtain information about the electronic behavior and whereas the electronic wave function of the system is localized or extended[9, 10]. Within this approach one can also obtain information about the fractality of the wave function and the criticallity of the system [11], and all these quantities can be measured experimentally [12].

In Fig. 5, we have the preliminary results for these calculations, we show the density of states of an approximant with $\sim 10^5$, and it agrees perfectly with others found in the literature[13, 14]. We calculate the typical density of states $\rho_{typ}(E)$ and compare it with the mean density of states $\rho_{me}(E)$ to look for energies where the electronic states are more localized (i.e where $\rho_{typ}(E) \ll \rho_{me}(E)$ and we found that the states in the center of the bands are more localized than the states at the
boundary. Finally we compute the probability distribution function to see its behavior is similar to the one expected for metals at the critical Anderson transition which is a log-normal behavior, however the preliminary results shows that the distribution seem to be more related to a bimodal distribution and this is something we are still trying to understand.
References


SCIENTIFIC REPORT

TEORIAS DE PARTICULAS FUNDAMENTAIS ALEM DO MODELO PADRAO.

Postdoc: Gero Freiherr von Gersdorff
Supervisor: Nathan Berkovits
FAPESP process: 2012/22639-0
Period: 01/04/2013 - 30/12/2015

[Signature]

[Signature]
Conferences and Seminars

- Invited Talk, May 2013, University of Mainz, Germany
- Participant and Collaboration, June 2013, GGI Institute, Florence, Italy
- Lecturer, September 2013, University of Sussex, Brighton, UK
- Talk, September 2013, WIN 2013 Conference, Natal
- Talk and Collaboration, September 2013, IIP, University Rio Grande do Norte, Natal
- Talk, December 2013, HEP 2013 Conference, Valparaiso, Chile
- Invited Plenary Talk, March 2014, Workshop: Hunting for a non standard Higgs sector, Benasque, Spain
- Invited Plenary Talk, May 2014, Planck conference, Paris, France
- Invited Lecturer, September 2014, BUSSTEPP summer school, University of Southampton, UK
- Invited Talk, September 2014, University of Helsinki, Finland
- Talk, November 2014, SILAFAE conference, Medellin, Colombia
- Invited Talk, Collaboration, May 2015, LPTHE/Jussieu, Paris, France
- Participant and Collaboration, September 2015, GGI Institute, Florence, Italy
- Invited Colloquium, November 2015, USP, São Paulo

Introduction

After completion of the first run of the LHC, we have started to probe physics responsible for electroweak symmetry breaking. The electroweak scale is many orders of magnitude lower than the Planck scale or the scale of a grand unified theory. For this reason, it is widely expected that new physics has to be present somewhere above the mass scale of the $W$ and $Z$ bosons. On the other hand, precision measurements at LEP have shown that the Standard Model (SM) accounts extremely well for all physics up to energies at least ten times the $W$ mass, providing strict bounds and constraints, and setting the scale of new physics around the Teraelectronvolt (TeV). It is thus a very challenging task to build actual models which explain the low scale of electroweak symmetry breaking (EWSB) without the necessity of severe fine tuning of parameters.

In 2012, the ATLAS and CMS experiments have announced the discovery of a new boson of mass $\sim 125$ GeV with properties consistent with the SM Higgs boson. The nature of the Higgs sector gives an excellent window to new physics, as almost all scenarios beyond the SM predict somewhat different Higgs couplings than the SM.
Research in 2013

The Higgs Boson as a Window to New Physics [1].

The SM predicts the couplings for all its particles to the Higgs boson. On the other hand, the LHC will be able to measure some of these couplings to a level of $\sim 5\%$ accuracy, which already allows us to put some limits on New Physics scenarios.

At present, the measured Higgs properties are consistent with the SM. In the diphoton channel there are however intriguing deviations at the 2$\sigma$ level which might well be due to statistical fluctuations or unknown systematics, or they might be the first sign of some New Physics coupling to the Higgs.

Given the trend of the data to coincide with the SM predictions, it seems justified to consider the hypothesis that New Physics states, if present, have masses considerably larger than the electroweak scale. For their impact on measurements at the Higgs mass pole it is then sufficient to integrate out these states. The resulting theory contains only SM particles and interactions, supplemented by a set of operators of dimension greater than four whose coefficients can be constrained. The large mass of the new states allows one to truncate the expansion in the dimension of the operators and only up to dimension six operators need to be considered. The effect of many higher dimensional operators (HDO’s) have been considered in relation with e.g. FCNC’s and electroweak precision data, and some of the coefficients are tightly constrained. Building on the success of this approach, my collaborators and I have performed a corresponding analysis for the Higgs properties [1].

The parametrization of New Physics by HDOs has several advantages over the conventional approach, in which each Higgs coupling is considered as a separate parameter, in particular it has fewer parameters and thus allows a correlation between the different couplings that in other approaches are unrelated.

We have used Bayesian inference which allowed us to easily marginalize over parts of the parameters space and to quote Bayesian Credible Intervals for all relevant operator coefficients. We have found that the HDO coefficients are already quite constrained, but still allow for certain deviations, in particular in the top Yukawa coupling as well as in the coupling of the Higgs to a photon and a Z boson.

Supersymmetric Models of Flavour [2].

Supersymmetry still remains one of the best motivated scenarios for a natural electroweak scale. Given the so far negative outcome of direct searches at the LHC, a certain tension has arisen, as heavy superpartners require more fine tuning for successful EW breaking. However, as has been realized a long time ago, only the top squarks and gluinos need to be light to avoid this situation, and one can have a perfectly natural scenario with heavier first two generation squarks. This scenario, in which only the states necessary for naturalness remain light, has been dubbed Natural Supersymmetry, and so far is not excluded by LHC limits (which mainly apply to the first two generation squarks).

FCNCs and CP violation are generically arising in all supersymmetric extensions of the
SM in which all or part of supersymmetry breaking is mediated by gravity, as the soft masses for the superpartners have no reason to be flavour-blind. It has been suggested that there might be a link to the spectrum of Natural Supersymmetry, as both from flavour physics and from direct searches the limits are the strongest for the first two generation superpartners. However, as bounds on flavour have improved, it has also become clear that a simple decoupling of the flavour problem (by multi-TeV first two generation squark masses) is not possible and some other flavour protection must be simultaneously present. One (obvious) such mechanism is a symmetry that suppresses mixing of squarks of different generations.

We have proposed a model [2] based on a family symmetry $G \times U(1)$, where $G$ is a discrete nonabelian subgroup of $SU(2)$, with both $F$-term and (abelian) $D$-term supersymmetry breaking. A good fit to the fermion masses and mixing is obtained with the same $U(1)$ charges for the left- and right-handed quarks of the first two families and the right-handed bottom quark, and with zero charge for the left-handed top-bottom doublet and the the right handed top. The model shows an interesting indirect correlation between the correct prediction for the $V_{ub}/V_{cb}$ ratio and large right-handed rotations in the $(s,b)$ sector, required to diagonalise the Yukawa matrix. For the squarks, one obtains almost degenerate first two generations. The main source of the FCNC and CP violation effects is the splitting between the first two families and the right-handed sbottom determined by the relative size of $F$-term and $D$-term supersymmetry breaking. The presence of the large right-handed rotation implies that the bounds on the masses of the first two families of squarks and the right handed sbottom are in a few to a few tens TeV range. The picture that emerges is light stops and left handed sbottom and much heavier other squarks.

Models of Flavour in Warped Geometries [3].

Warped extra dimensions, or Randall Sundrum (RS) models, are a very interesting alternative explanation for a natural electroweak scale. Moreover, they incorporate an explanation of the fermion mass hierarchy observed in nature, without relying on very small Yukawa couplings. Instead, suppression factors appear naturally as exponentially suppressed wavefunction overlap integrals. The very same suppression factors also tame the dangerous FCNCs.

In recent paper [3] I have reviewed the bounds on these models arising from both hadronic and leptonic physics. The strongest bound originate from neutral meson mixing and from $\mu \rightarrow e\gamma$ rare decays, both pointing to a Kaluza Klein scale in the range $\sim 20$ TeV and above. Baring fine-tuned scenarios, the RS flavour paradigm needs to be supplemented with additional FCNC suppression mechanism such as symmetries or a modified geometry.

Anomalous Gauge Couplings [4].

Yet another set of SM couplings that can be studied at the LHC at high precision are the gauge-boson self interactions. In particular, neutral quartic gauge boson self interactions are highly suppressed in the SM and are hence a particulary interesting window to New Physics.
Such effective interactions are mediated only by dimension-8 operators, and thus to probe them one needs energies much larger than the EW scale, attainable at the LHC.

In a recent paper [4] we have studied the generation of such couplings in a series of well-motivated extensions of the SM, such as composite Higgs models and models with warped extra dimensions. We derived the general perturbative contributions to the pure field-strength operators from spin 0, $\frac{1}{2}$, 1 resonances by means of the heat kernel method. In the composite Higgs framework, we derived the pattern of expected deviations from typical $SO(N)$ embeddings of the light composite top partner. We then studied a generic warped extra dimension framework with $AdS_5$ background, recasting in few parameters the features of models relevant for anomalous gauge couplings. We also presented a detailed study of the latest bounds from electroweak and Higgs precision observables, with and without brane kinetic terms. We have found that, for vanishing brane kinetic terms, EW precision observables require KK masses of at least 6 TeV, even in models where custodial symmetry suppresses the $T$ parameter. We also presented a detailed study of these constraints in the presence of brane kinetic terms. While this allows one to relax the constraints from EW precision tests, anomalous gauge couplings are unsuppressed in this region of parameter space, and can provide dominant constraints.

**Research in 2014**

**New physics from light-by-light scattering at the LHC [5, 6].**

Indirect probes of New Physics can be powerful if the SM process is strongly suppressed. This happens in scattering of light by light, which in the SM can occur via loops of quarks, leptons and the $W$ boson. Due to the smallness of the electroweak coupling it is strongly suppressed. New Physics contributions can arise in two different ways, either from charged particles, or from neutral ones with couplings to the field strength tensor. In the former case, strong enhancements can occur in New Physics scenarios with very large electric charges. The effect is largely model-independent, as it only depends on the electric charges of the new particles and their spin, whereas other couplings/details of the model do not matter at all.

Light-by-light scattering can be measured at the LHC via so-called diffractive processes, in which the protons emit (almost) on-shell photons of energies in the range 200-1000 GeV. The scattered protons remain intact and can be detected in specially designed detectors installed close to the beam pipe in the forward region of the Atlas and CMS central detectors. This allows a precision measurement of the kinematics of the event, which in turn offers a very efficient way to reject backgrounds.

We have performed a detailed study of the sensitivity to the presence of new charged and neutral particles. We find that these experiments will be able to place model-independent bounds on charged particles that are more stringent than with other precision measurements, including the $g - 2$ measurement of the muon. Moreover neutral particles of spin 0 and 2 (such as dilaton and the Kaluza Klein graviton) can be excluded in the multi TeV range, if sufficiently strongly coupled.
The Dynamical Composite Higgs model [7]

The Higgs as a composite Goldstone boson is one of the prime candidates for a natural mechanism of EWSB. However, the dynamics of the global symmetry that gives rise to these Goldstone bosons has not been studied in detail. It has been known for a long time that a symmetry can be broken in a purely fermionic theory in the presence of a sufficiently strong four-fermion interaction. We apply this so-called Nambu-Jona-Lasinio (NJL) model to the breaking of the $SO(5)$ symmetry of typical composite Higgs models. The NJL model is extremely predictive, as the low energy couplings of the emerging composite scalars are determined by a characteristic fixed-point behaviour of the renormalization group. In the context of the composite Higgs model, this results in highly predicted spectrum of resonances of spin 0, 1/2 and 1, which can be tested at the LHC.

Research in 2015

Radiative corrections from higher spin fields [8]

It is known that contributions from charged particles in loops grow quite fast with the spin, as has been shown in the case of $s \leq 1$. If this behaviour remains true for larger spin, light-by-light scattering might constitute an interesting probe for the presence of higher-spin particles, like string excitations or strongly-interacting bound states. Further tools are however necessary to handle quantum computations involving higher-spin particles. We are in the process of developing a formalism to deal with loops of particles of spin $\geq 2$.

Effective Theory for Diboson Signals [9]

We have classified the complete set of dimension-5 operators relevant for the resonant production of a SM singlet of spin 0 or 2 coupled to the SM. We computed the decay width of such states as a function of the effective couplings, and provide the matching to various well-motivated New Physics scenarios. We investigated the possibility that one of these neutral resonances be at the origin of the excess in diboson production recently reported by the ATLAS collaboration. We performed a shape analysis of the excess under full consideration of the systematic uncertainties to extract the width $\Gamma_{\text{tot}}$ of the hypothetical resonance. We then point out that the three overlapping signal regions reported by ATLAS follow a joint trivariate Poisson distribution, which opens the possibility of a thorough likelihood analysis of the event rates. The background systematic uncertainties are also included in our analysis. We then use both the information on the width and the cross section, which prove to be highly complementary, to test the effective Lagrangians of singlet resonances. Regarding specific models, we find that neither scalars coupled via the Higgs-portal nor the Randall-Sundrum (RS) radion can explain the ATLAS anomaly. The RS graviton with all matter on the infrared (IR) brane can in principle fit the observed excess, while the RS model with matter propagating in the bulk requires the presence of IR brane kinetic terms for the gauge fields.
Scientific Report 2015

Pesquisa em AdS-CFT correspondence
Física das Partículas Elementares e Campos

Postdoc : Chrysostomos Kalousios
Supervisor : Nathan Jacob Berkovits
FAPESP
Process : 2012/00756-5
Period: 01/01/2015 - 30/9/2015

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Service and Outreach

Referee for JHEP.

Invited talks, Presentations and Workshops in 2015

Participant in “Program on Integrability, Holography and the Conformal Bootstrap”, ICTP, São Paulo, Brazil, November 1-February 28, 2015.

Participant in “3rd Joint Dutch-Brazil School on Theoretical Physics”, ICTP, São Paulo, Brazil, February 2-6, 2015.

Invited talk, University of Cape Town, Cape Town, South Africa, May 28, 2015.

Invited talk, University of the Witwatersrand, Johannesburg, South Africa, June 2, 2015.

Invited talk, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing, China, June 30, 2015.

Invited talk, Interdisciplinary Center for Theoretical Study, University of Science and Technology of China, Hefei, China, July 9, 2015.

Participant in “School on QCD and LHC Physics”, ICTP, São Paulo, Brazil, July 22-31, 2015.

Invited talk, National Taiwan University, Republic of China, September 11, 2015.

Invited talk, National Center for Theoretical Sciences, National Tsing-Hua University, Hsinchu, Republic of China, September 14, 2015.
Publications in 2015


Published work

Work on soft theorems [1]

Construction and studies of soft theorems, that is the behavior of an amplitude when one of the external particles becomes soft, play an important role in the study of a scattering process. Besides serving as a test for higher point amplitudes, sometimes it can be also used in order to construct the full amplitude of the theory.

Recently, Strominger proposed that a certain infinite-dimensional subgroup of the BMS (Bondi, van der Burg, Metzner, Sachs) supertranslation group is an exact symmetry of the quantum gravity $S$-Matrix [2]. Weinberg’s soft theorem [3, 4] is a Ward identity for this subgroup [5].

It was further conjectured by Cachazo and Strominger [6] that there is a new universal soft graviton theorem which is valid up to next to subleading order in gravity, whose precise formulation can be found in the original reference. One of the natural questions I asked and together with Francisco Rojas we studied in [1], was whether the aforementioned theorem is valid to an arbitrary number of dimensions. Indeed, the starting point was the Cachazo-He-Yuan formalism [7] and after a long computation we were able to establish the Cachazo-Strominger theorem in arbitrary dimensions. One of the surprises is the fact that the original soft theorem was based on the BMS symmetry, which is only available in four dimensions.

Work on the computation of scattering amplitudes [8]

In [9] it was argued that the tree level S-matrix of massless theories can be captured by the so-called scattering equations that connect the space of kinematic invariants of $n$ particles in arbitrary spacetime dimensions to the positions of $n$ points on a sphere.

One of the questions is how to use the formalism in order to get explicit answers for the amplitudes. Some attempts have appeared in the past and involved special solutions of the equations associated to particular polynomials, that in some of the cases allowed for the explicit construction of the amplitude. Besides all the efforts there is no known general solution of the scattering equations.

Fortunately, one does not need to know the explicit solutions of the equations in order to evaluate the amplitude. The amplitude is always given as sums of all possible solutions of the scattering equations, which are polynomial in nature, and one can then use the well known in mathematics formulas of Vieta, that associate the sums of roots of polynomials to the coefficients of these polynomials. This can be the first step, but still the answer is complicated to evaluate and write it down.

In this work I presented an algorithm that in principle allows the explicit evaluation of any tree level amplitude in terms of kinematic invariants. I then used the method to explicitly evaluate all five point amplitudes.

Submitted for publication

Comments on the scattering equations [10]

In this work Carlos Cardona and I used presented three computations related to the explicit evaluation of scattering amplitudes.

The first computation is a simple and interesting rewriting of the most general integral in the $n = 5$ case. This integral that depends on five cross ratios was previously evaluated in [8] through the construction of a generating function that gives integrals raised to different powers of the cross ratios. In this work we gave an alternative expression of the aforementioned fundamental quantity purely in terms of Chebyshev polynomials, by employing properties of the polynomials and making use of the fact that for $n = 5$ the scattering equations have two solutions.

The second computation is for general $n$ and special kinematics. Studying amplitudes at special kinematics is definitely interesting as it reveals features of the scattering equations and the amplitudes that are hidden in the complexity of the general solutions. Motivated by this, we considered a special kinematics that allowed the linearization of the polynomial in nature scattering equations. Then, any
amplitude can be straightforwardly evaluated without the need to know the explicit solutions of the scattering equations.

The third computation is related to the method of companion matrices. We provided several comments and argued that the method is equivalent to the elimination theory of \[11\] and an algorithm presented by one of the authors in \[8\]. The basic idea is that because of the explicit form of the companion matrices, evaluating any given amplitude by taking traces of companion matrices is essentially a neat way to isolate the appropriate coefficients of polynomials that the scattering equations satisfy. The latter was also the observation in \[8\], where the coefficients of polynomials were put in use through the well-known in mathematics Vieta formulas.

### Research plan

I am submitting my research plan because I have applied for a renewal of my process.

### Geometrical structures of scattering amplitudes

It is well known by now that massless scattering can be described through the sum of roots of a rational function with variables that satisfy the so-called scattering equations. In their general form the scattering equations can be viewed as a multilinear system of polynomial in nature equations. Unfortunately, we cannot obtain explicit solutions of this system in view of the Abel-Ruffini theorem. Fortunately though one does not need to do so, but instead can use the coefficients of the scattering equations in order to read off the scattering amplitudes. In order to achieve this one needs to know two ingredients. First how to write the scattering equations as a one variable polynomial and second how to write the rest of the variables of the scattering equations in terms of one variable. Then the scattering amplitudes is reduced to a one variable polynomial whose sum over roots follows the well-known Vieta formulas. Carlos Cardona and I are currently working on this problem that comes by the name of elimination theory. The results that we have obtained so far suggest that such a construction is possible and can be achieved in various equivalent ways each one exhibiting different features of the elimination and the final answer takes the form of a determinant that satisfies on-shell recursion relations.

From the structure of the aforementioned determinant one can see that the scattering equations exhibit a combinatorial structure that can perhaps be captured through geometrical structures. The goal here would be to uncover these structures and then use them in order to describe scattering amplitudes using geometry. The idea that scattering amplitudes can be described via geometry is not old, with some recent examples referring to the construction of the amplituhedron \[12\]. Since the scattering equation description is valid in arbitrary dimensions and for several different theories it would be interesting to attempt a geometric understanding of the amplitudes the way we described. Finally it would be interesting to relate the two seemingly orthogonal descriptions of amplitudes, the scattering equation framework and the amplituhedron.

### Explicit evaluation of scattering amplitudes

Using the elimination theory described in the previous section one can in principle evaluate any given amplitude that satisfies the scattering equations, such as pure Yang-Mills, gravity, etc via pure algebraic manipulations the only limitation being computer power. The final answer is given in terms of kinematic invariants formed out of momenta and helicities of the external particles and it is valid in arbitrary spacetime dimensions. Due to the importance of having explicit results of amplitudes both for phenomenological as well as theoretical purposes one would like to know explicit expressions of them. We have achieved our goal using the elimination theory, but we believe one can do even better. The elimination theory is very general and it can be applied to a sum of any arbitrary rational function, not necessarily constrained to be related to scattering amplitudes. We believe that if one specializes elimination to scattering amplitudes he will be awarded with huge calculational simplifications that not only they will help with algebra, but in some cases they might even allow for the explicit construction of the amplitudes in terms of compact expressions that contain structures like determinants and pfaffians.
Bibliography


Scientific report 2015

Probing the large scale structure of the universe with Planck and the Dark Energy Survey

Postdoc: Fabien Jean-François LACASA
Supervisor: Nathan Jacob Berkovits
FAPESP
Process: 2013/19936-6
Period: 1/12/2013 - 30/12/2015

ICTP-SAIFR
Sao Paulo
Scientific report 2015

Fabien Lacasa

I joined ICTP-SAIFR on December 1st 2013.
I immediately joined the Dark Energy Survey Collaboration, working with Prof. Rogerio Rosenfeld.
I retained my membership in the Planck Collaboration and participated to the 2015 release.
I started this year co-supervising undergraduate student Nickolas Kokron (bolsa FAPESP de Iniciação Científica) together with Prof. Rogerio Rosenfeld.

1 Presentations

1.1 In conferences or workshops

Poster
- May 25th-29th 2014 poster in IAU Symposium 306 in Lisboa (Statistical Challenges in 21st Century Cosmology) : Combining cluster counts and galaxy clustering probes

Talks
- January 28th 2015 at Cosmology on Safari (Bonamanzi, South Africa) : Non-Gaussian tools for the Large Scale Structure
- May 24th 2015 at VIth WORKSHOP CHALLENGES OF NEW PHYSICS IN SPACE (Campos do Jordao, Brasil) : Combining probes : cluster counts and galaxy power spectrum

1.2 DES Collaboration meetings

- May 12th 2015 at DES-Michigan : Combining probes : cluster counts and galaxy power spectrum
- October 6th 2015 at DES-Madrid : Combined probes : cluster counts and galaxy C(l) + DES-Brazil updates
- October 8th 2015 at DES-Madrid : Covariance of clusters and galaxies : comparison with MICE

1.3 Seminars

2013
- December 2nd 2013 at USP : Non-Gaussianity and foregrounds to the CMB

2014
- February 21st 2014 at ICTP-SAIFR : Non-Gaussianity and extragalactic foregrounds to the CMB
- March 17th 2014 at ICTP-SAIFR : CMB polarization B modes and primordial gravitational waves
- March 25th 2014 at USP : Primordial gravitational waves and CMB polarization
- April 8th 2014 at USP : Non-Gaussianity, galaxies and clusters
- April 14th 2014 at USP : Combining probes of the large scale structure

\[ http://sccc21.sim.ul.pt/ \\
\[ http://www.acru.ukzn.ac.za/~cosmosafari/ \\
\[ https://vichallenges.if.ufrj.br/ \\
\[ http://desmichigan.lsa.umich.edu/home \\
\[ https://workshops.ift.uam-CSIC.es/desmeetingmadrid \]
2015
- February 4th 2015 in UKZN Durban : Non-Gaussianity with Planck and DES
- April 14th 2015 at Institut d’Astrophysique de Paris (Paris, France) : Combining probes : cluster counts and galaxy power spectrum
- April 20th 2015 at AstroParticule et Cosmologie Laboratory (Paris, France) : Combining probes : cluster counts and galaxy power spectrum
- April 21st 2015 at Institut d’Astrophysique Spatiale (Orsay, France) : Combining probes : cluster counts and galaxy power spectrum
- October 15th 2015 at Commissariat à l’Energie Atomique (Saclay, France) : Combined probes : cluster counts and galaxy C(l)

2 Publications

This pdf hyperlink should get you to a list of most of my publications on the NASA Astrophysics Data System (ADS). This other pdf hyperlink gets you to my publication list on inSPIRE, which is a bit more complete.

Publications from the start of the FAPESP fellowship until now :
- Planck 2015 results. I. Overview of products and scientific results arXiv:1502.01582, ADS link
- Planck 2015 results. XVII. Constraints on primordial non-Gaussianity arXiv:1502.01592, ADS link
- Planck 2015 results. XXII. A map of the thermal Sunyaev-Zeldovich effect arXiv:1502.01596, ADS link
- Scaling of the 1-halo terms with bias arXiv:1506.02315, ADS link
- Combining cosmological constraints from cluster counts and galaxy clustering arXiv:1407.1247, ADS link

3 Supervision

I co-supervise, together with Prof. Rogerio Rosenfeld, undergraduate student Nickolas Kokron from USP Ciencias Moleculares for his two-year project Iniciacao Cientifica entitled : "Medindo o Espectro de Potencias Angular em Leventamentos Astronomicos Cut-Sky"

4 Research statement

4.1 Introduction

In the last decades, cosmological and astronomical observations have brought up three of the most important challenges of 20th century physics : inflation, dark matter and dark energy. Current and future observations of the large scale structure of the universe are and will be providing clues on those puzzles, most possibly fostering new understandings of particle physics and gravity.

My scientific goal is to develop data analysis methods and the corresponding theoretical modelisation, in order to extract as much information as possible from large scale structure observables, and thus maximize the scientific output of cosmic surveys.

To this end, I am interested in Bayesian inference, high order statistics of cosmic fields and combined probes. I develop estimation tools for data analysis, especially non-Gaussianity, apply them to current
surveys (Planck, Dark Energy Survey), and develop modelisation at the necessary non-linear level, with the halo model and adapted extension.

Note: in the pdf file, hyperlinks to my publications are given throughout the text.

4.2 non-Gaussianity and combined probes for Planck and DES

Non-Gaussianity, Cosmic Infrared Background and thermal Sunyaev-Zel’dovich effect in Planck

I am a member of the Planck Collaboration, an experiment mapping the microwave sky from 30 to 857 GHz with primary driver to map the anisotropies of the Cosmic Microwave Background (CMB). I worked on non-Gaussianity (NG), the Cosmic Infrared Background (CIB) and the thermal Sunyaev-Zel’dovich (tSZ) effect.

To study non-Gaussianity of the spherical microwave maps, I focussed on the angular bispectrum, the connected three-point correlation function of spherical harmonic coefficients. I adopted the binned bispectrum estimator, and also used the KSW estimator (Komatsu et al. 2005), a contraction of the bispectrum purposely built to search for primordial CMB NG.

I participated in the Planck working group on primordial non-Gaussianity, assessing the level of non-Gaussianity contamination by extragalactic point-sources (Planck 2013 and 2015 results), and my own CIB NG estimation method (developed previously in Lacasa et al. 2014a) was used in the 2015 results.

Non-Gaussianity can also be useful to constrain the physics of the CIB, which probes both the star formation history and the large scale structure of the universe at high redshifts. That is why I started, already during my PhD, a collaboration with Dr. Aurélie Pénin (UKZN South Africa) and undertook the effort of modeling the CIB bispectrum with the halo model, Halo Occupation Distribution (HOD) and a model of the global IR emissivity history, characterising this bispectrum and forecasting its sensitivity to model parameters : [Lacasa et al. 2014b] and [Pénin et al. 2014]. I also undertook during my PhD the measurement of the CIB bispectrum in Planck data in CIB estimated maps, cleaned from the CMB and galactic dust contamination. The results are presented in the Planck 2013 CIB article.

Surprisingly, the measured bispectrum is significantly steeper than both the phenomenological prescription and the previously-presented physical modelisation. The current interpretation is that it is the sign of host dependence of IR emissivity, since the quenching of star formation in massive halos should suppress power on small non-linear scales. That is why Dr. Pénin and myself are currently developing a bispectrum model accounting for this effect via a variant of sub-halo abundance matching (SHAM) and intend to constrain the model by MCMC comparison with Planck data. I was invited to visit UKZN (Durban South Africa) in January 2015 following a conference in Bonamanzi, and Dr. Aurélie Pénin was invited to visit ICTP-SAIFR in February-March 2015, in order to pursue our collaboration. These works should result in a 2016 publication (Pénin, Lacasa, Ilić, in prep.).

I have also studied the non-Gaussianity of the thermal Sunyaev-Zel’dovich effect (tSZ). This signal comes from the Thomson scattering of CMB photons off free electrons in the hot ionised gas of galaxy clusters, with an amplitude dependent on the electron pressure and density but independent of redshift. Thus, it probes massive halos and gas physics up to redshifts inaccessible to other probes. The tSZ effect is very non-Gaussian, so that the bispectrum contains significant additional information compared to the power spectrum. I undertook the measurement of the tSZ bispectrum on Planck data, using internal component separated maps. The measurement was complicated by the mask effect, leaking power from large to small scales, which proved to be much more significant than for the CIB due to the tSZ bispectrum being steeper. To tackle this mask effect, several methods were studied in my PhD thesis. For the Planck measurement, I constructed devoted non-Gaussian simulations to invert this effect and discard configurations were it was too strong. I performed the measurements for the Planck 2015 data release, and they proved to be of high quality with a
conservatively-estimated significance of 60 $\sigma$. A full-fledged interpretation of the measurement would require a physical bispectrum model, which was not available at the time of the Planck 2015 release. I am currently precisely working on such a modelisation, in collaboration with Dr. Guillaume Hurier (CEFCA Spain), Dr. Nabila Aghanim and Dr. Marian Douspis (IAS Orsay France). (Hurier and Lacasa, in prep.) and the subsequent cosmological constraints inferred from the comparison of the model and Planck measurement.

### Halo modeling and Dark Energy Survey

I am also involved in analysis and modelisation for galaxy surveys data, and have joined the Dark Energy Survey Collaboration, a photometric optical survey of the Southern sky. I am working on using the halo model and HOD to describe galaxies and clusters, as well as developing estimation on DES data.

I have worked with Prof. Raul Abramo and collaborators (USP São Paulo) in investigating how the non-linear part of the power spectrum scales with galaxy bias : Abramo et al. 2015. Indeed, using the halo model and HOD, both $P_{1h}$ and $b_{gal}$ can be predicted from HOD parameters. We found an interesting scaling $P_{1h} \propto b_{gal}^{-4.5}$, which we also generalised to higher orders : 1-halo bispectrum, trispectrum etc. This scaling is steeper than the one of the linear power spectrum, $P_{2h} \propto b_{gal}^2$, so that it puts into question the use of arbitrarily highly biased tracers for cosmological analysis. It also puts into question the use of a fixed non-linear template, e.g. HALOfit (Peacock and Smith 2014), to predict the power spectrum of different galaxy populations.

Within DES, my main project is to combine constraints from two probes of the large scale structure : the cluster number counts and the galaxy angular power spectrum, or equivalently the angular correlation function. To this end, we need to compute the joint covariance of these probes, in particular the cross-covariance which is a 3-point function ; it also turns out critical to incorporate non-Gaussianity in the power spectrum covariance, i.e. the trispectrum. Some preliminary results are given in the proceeding of the IAU S306, and a full-fledged analysis should be submitted soon (Lacasa and Rosenfeld 2015, in prep.). I have started a collaboration with Dr. Kai Hoffmann and Dr. Enrique Gaztañaga (ICE Barcelona) in order to compare this theoretical prediction of the joint covariance matrix with the MICE-GC N-body simulations. Dr. Kai Hoffmann was indeed invited to stay at ICTP-SAIFR São Paulo for three months in 2015.

Finally, I am involved in various DES or DES-Brazil projects, in particular on questions of statistical analysis, estimation and halo modeling : DES year 1 HOD and BAO analyses, covariance of cluster counts and multi-probe analysis for the problem of super-sample covariance. I am co-supervising with Prof. Rogerio Rosenfeld (UNESP São Paulo) a project from undergraduate student Nickolas Kokron, estimating galaxy angular power spectrum on MICE-GC and DES data. I am also currently working on an HOD modelisation of the covariance of the galaxy angular power spectrum, including all numerous non-Gaussian terms and effects : perturbation theory, super-sample covariance, shot-noise, second order biases, non-local tidal effect...

## 5 Proposed research for 2016 : optimal analysis of galaxy and cluster distribution

The first item of my future research is of course to continue my fruitful participation in my current collaborations and further develop the projects I have described, taking part in particular in the Planck 2016 release and future DES releases.

Beside these works, I envision three main additional axes for my research.

### Combined probes for galaxies and clusters

I am interested in investigating the full information contained in galaxy and cluster 1- and 2-point statistics, in order to optimally analyse galaxy clustering. That is, combining all these probes : galaxy...
and cluster counts, auto and cross power spectra, in order to investigate where the information comes from and if some probes can be dropped for practical purposes. To this end I propose to model the full covariance with the halo model, including in particular all non-Gaussian contributions and super-sample covariance (SSC).

**Halo modeling of the large scale structure**

I would like to develop large scale structure modelisation with the halo model, and in particular understand why it fails at the moment on intermediate mildly non-linear scales, and to find out how to solve this problem. In my opinion, the problem could involve the effects of non-local halo bias (tidal force effect), asphericity and/or alignment of halos, voids, filaments and walls, or other phenomenologically unaccounted physics. I think that comparison with perturbation theory and with dark matter N-body simulations will be of prime importance to understand this problem.

I would also explore the assignation of galaxies into halos, current methods being halo occupation distribution (HOD), conditional luminosity function (CLF) and sub-halo abundance matching (SHAM). For instance, Pujol et al. 2015 have shown that the galaxy number correlates much better with background density than with halo mass, rendering HOD approaches suboptimal and potentially biased. It would be particularly interesting to combine these methods with my diagrammatic formalism introduced in [Lacasa et al. 2014b] so as to predict multi-tracers and/or multi-types statistics. The latter is indeed a promising approach to extract more information from cosmological modes, beating down cosmic variance (e.g. Abramo et al. 2013, 2015).

**Alternative analysis methods of galaxy and cluster distributions**

I will explore alternative decomposition bases to treat galaxy survey observables, such as the Fourier-Bessel basis which is better adapted to treat spectroscopic or semi-spectroscopic survey, e.g. PAU or JPAS, than the usual 3D Fourier basis or the angular statistics per redshift bin. This will be particularly interesting to produce an optimal treatment of redshift-space distortions.

I am keen on exploring other statistics for the galaxy and cluster density field, additions to the power spectrum. The bispectrum in particular has been shown to carry a lot of information about cosmology and galaxy formation (e.g. Sefusatti 2005). This is a statistic I have experience with and is particularly useful to uncover effects which are subdominant in the power spectrum, for instance higher order perturbation theory and non-linearity and non-locality in halo biasing. I will research bispectrum methods which are numerically tractable for current and next generation surveys, and investigate the information content of the bispectrum compared to the power spectrum. That is, how much additional information is present in a joint analysis, which bispectrum modes carry the most information, and what level of modelisation is needed for a precise covariance matrix. For the latter I will explore the importance of non-Gaussian and shot-noise term via my diagrammatic formalism. I will also investigate the implementation of the bispectrum measurement on data: linear correction term, mask effect, mitigation of systematics, implementation in the Fourier-Bessel basis.

Moreover, I will explore the $A^*$ statistic proposed by Carron et al. 2014a, which is supposed to extract all the information of the galaxy density field, in the log-normal model. This statistic is however agnostic to the knowledge of clusters and the structuration of matter in general as well as to perturbation theory knowledge of gravitational collapse. It will thus be interesting to compare the additional information uncovered by $A^*$ compared to the joint analysis of galaxy and detected clusters 1- and 2-point moments, as well as joint analysis with the bispectrum.

Finally, I will explore how to best use the detection of clusters and their characteristics determination. For instance, one could mask out the clusters with robust mass determination from the galaxy catalog, and implement a joint analysis of the rest of the galaxies with the cluster sample. At two-point level, that would involve the power spectrum of the unmasked galaxies, the cluster power spectrum per mass bin, and the diverse cross-spectra between the samples. Such analysis should reveal the signal from less massive clusters and/or lower density environment, which would otherwise be
buried in the cosmic variance of the massive clusters signal. Again, I could use the background density proposed by Pujol et al. 2015 instead of halo mass, as well as other measured halo informations, as long as the corresponding determinations are robust and have well-defined selection functions.
SCIENTIFIC REPORT

SCHOLAR: Saeed Mirshekari, FAPESP Postdoctoral Research Fellow, ICTP-SAIFR
SUPERVISOR: Nathan Berkovits, Professor do Instituto de Fisica Teorica, UNESP

October 22, 2015

SAEED MIRSHEKARI, 22 October 2015

Nathan Berkovits

Oct 22, 2015
This is a report in which I briefly review my research projects as a FAPESP Postdoctoral Research Fellow at ICTP-SAIFR during September 2013 - Jun 2015. The results, publications, and other professional activities on these research projects during this period of time are also listed in this report. This report is requested by FAPESP to submit as the final scientific report on the contract number 2013/14754-7 between FAPESP organization, Nathan Berkovits as the supervisor and Saeed Mirshekari as the FAPESP research fellow.
Chapter 1

Research Projects

1.1 GW Data Analysis: Testing The Accuracy of GW Searches

1.1.1 Summary and Initial Plan

The completion of upgrades and starting the first scientific run (September 2015) of the kilometer-scale, laser interferometric gravitational-wave (GW) observatories in the U.S. (LIGO) holds the promise to open a new astronomical window in to the high-frequency GW band. Since GW signals are extremely weak compared to the background noise, an accurate data analysis is crucial to extract the buried GW signals from the noisy data. An accurate data analysis provide a mechanism to study the physical properties of the astronomical GW sources. Our initial plan for this research project at ICTP-SAIFR was developing a comprehensive test mechanism for testing the consistency and accuracy of the numerical and analytical gravitational-waves templates with and without some extra features such as spin precession, amplitude correction terms, and waveform bias. The initial plan for this research was quantifying the accuracy of one of the main search pipelines in data analysis group at LIGO, i.e. PyCBC, in different regimes under various conditions.

1.1.2 Progress and Accomplishments

Following the initial plan, as a part of reviewing current available Post-Newtonian waveform approximants to be used in LIGO gravitational-wave searches, we investigated the effect of (A) spin precession, (B) amplitude corrections and (C) waveform bias on the modeling accuracy of gravitational waves emitted by compact binary systems. We quantified our study by showing how faithfulness, effectualness, and parameter bias are affected by factors A, B and C (and any combinations of them). A catalogue of results has been obtained. The numerical calculations has been done mainly through PyCBC toolkit of LIGO Scientific Collaboration (LSC). In this comprehensive study, we considered both inspiral-only waveforms (spin-aligned TaylorF2 and SpinTaylorT4) and inspiral-merger-ringdown waveforms (IMRPhenomP, SEOBNRv2 and PhenSpinTaylorRD) and the method we developed is applicable to other wave-form templates as soon as they become available (IMRPhenomD, for instance). Novel results have been obtained and wherever comparison is possible, we found complete agreement with previous studies. The research activities in this sector have been under the Compact Binary Coalescence (CBC) group and the Waveform subgroup of LSC.

ICTP-SAIFR gravitational-waves data-analysis research group had a significant contribution to the LIGO Scientific Collaboration (LSC). ICTP-SAIFR joint LSC in October 2013. The members include Riccardo Sturani (PI) and Saeed Mirshekari. Our research proposal to join LSC have been presented and accepted by LSC’s committee at LVC meeting at Nice in September 2013. Preliminary results have been presented at annual LIGO-Virgo Collaboration meeting in Stanford, August 2014 and at NARDA meeting at California State University, Fullerton in 2014. During this period of time in which I was working on this project I had a chance to visit the Center for Gravitation and Cosmology (CGCA) at University of Wisconsin-Milwaukee.
twice in 2014 in January and September and LIGO Lab at Caltech Institute of Technology in March 2015.

The last updated results of this research project have been presented at annual APS meeting, April 2015 and in Caltech Institute of Technology in March 2015. The first draft of the results for publication has been submitted to the head of the research group at ICTP-SAIFR, R. Sturani, for his review and comments in November 2014 and has been updated since then constantly up to it’s final stages in Jun 2015. This draft paper will be improved and prepared for publication by R. Sturani soon (S. Mirshekari’s contract was canceled unilaterally by FAPESP in Jun 2015 because of the absence of the fellow at ICTP-SAIFR site for family emergencies after he left Brazil to USA for a work conference in late April. His request for working remotely for the last two months of his contract got denied by FAPESP’s committee based on this organizations’ policies).

In addition to above project, since 2014 I also contributed to work on a project focused on parameter estimation of gravitational wave sources in collaboration with my mentor at ICTP-SAIFR R. Sturani and our colleagues at University of Birmingham, UK i.e. Alberto Vecchio, John Veitch, and Walter Del Pozzo. The proposal of this collaborative project between the research groups at ICTP-SAIFR and University of Birmingham has been approved to get funded by FAPESP and University of Birmingham via contract #2014/50259-3 for 2 years (PI: Riccardo Sturani).

1.2 Alternative Theories of Gravity

1.2.1 Summary and Initial Plan

Although Einstein’s General Theory of Relativity has successfully passed all the experimental tests so far up to a very good level of accuracy, this theory is not the only valid theory of gravity. There are also several other competitive theories which are in agreement with all observation as well as for Einstein’s theory. However, the theory of gravity has not been tested in strong gravitational field regime such as in a regime close to compact celestial objects like a black-holes and neutron stars. In these extreme gravity regimes the predictions of different theories are recognizably different. Gravitational waves emitted from such copact objects provide us a great testbed to test the theories of gravity. Scalar Tensor Theories of Gravity are the simplest and the most popular alternative theories of gravity.

A broad class of classical relativistic field theories of gravity containing $N$ finite-range scalar fields and a metric tensor, and satisfying the Weak Equivalence Principle, can be constructed in both the Jordan and Einstein frames in a target-space-covariant manner (the weak-field limit of tensor-multi-scalar theories has been worked out in [2]). The field equations can be cast into both hyperbolic form suitable for numerical integration, and relaxed harmonic form suitable for Post-Minkowskian (PM) and Post-Newtonian (PN) expansions. We have successfully checked the consistency of our results for the case of a single scalar field ($N = 1$) with the previous results [3].

A tensor-bi-scalar theory of gravity with spherical target-space geometry is explicitly constructed. This theory passes solar-system and binary-pulsar tests, and contains an unconstrained parameter, namely, the target-space curvature, which enters at higher Post-Newtonian orders into the waveform emitted by a compact-binary-inspiral. Potential bounds on this parameter coming from future gravitational wave observations can be made. This work was in collaboration with Michael Horbatsch, Emanuele Berti, and Hector O. Silva at University of Mississippi.
1.2.2 Progress and Accomplishments

Given that my PhD work have been dedicated to modeling and testing Scalar Tensor Theories of Gravity as one of the most popular class of alternative theories of gravity, I carried on and continued this research stream-line to ICTP-SAIFR and worked closely with my colleagues at University of Mississippi on a project studying multiple scalar tensor theories of gravity since my first days in ICTP-SAIFR in 2013. A significant part of this collaboration was a result of participating in a workshop at University of Mississippi in January 2014, Oxford MS. With Emmanuelle Berti from University of Mississippi and a group of authors, I actively contributed to writing a refereed review paper on this subject titled "Testing General Relativity with Present and Future Astrophysical Observations" accepted for publication in Classical and Quantum Gravity, 2015.
Chapter 2

Outcomes as FAPESP scholar

Here in this chapter, the journal publications, delivered seminar talks, and professional experiences of mine affiliated as the FAPESP postdoctoral research fellow in various journals and professional events from September 2013 are listed.

2.1 Journal Publications

- “A Directed Search for Gravitational Waves from Scorpius X-1 with Initial LIGO”, LIGO Scientific Collaboration and Virgo Collaboration, Phys. Rev. D 91 (6), 062008, 2014
- “Advance LIGO”, LIGO Scientific Collaboration and Virgo Collaboration, Class. Quantum Grav. 32 (7), 074001, 2014

2.2 Delivered Seminar Talks

- APS April Meeting, Baltimore MD, April, 2015
- Caltech Institute of Technology, Pasadena CA, March, 2015
- ICTP-SAIFR Workshop on Observational Cosmology, São Paulo, Brazil, December, 2014
- LVC Meeting, Stanford University, Paulo Alto CA, August, 2014
- NARDA Meeting, California State University, Fullerton CA, August, 2014
- University of Wisconsin-Milwaukee, Milwaukee WI, January, 2014
- ICTP-SAIFR, São Paulo State University, Brazil, November, 2013
2.3 Professional Experience

2.3.1 Visiting Research Scholar

- Caltech Institute of Technology, Pasadena CA, March 20–27, 2015
- University of Wisconsin-Milwaukee, Milwaukee WI, September 1–30, 2014
- University of Wisconsin-Milwaukee, Milwaukee WI, January 13–February 5, 2014

2.3.2 Conferences and Meetings

- APS April Meeting, Washington DC, April 11–14, 2015
- LIGO-Virgo Meeting, Caltech Institute of Technology, Pasadena CA, March 15–19, 2015
- LIGO-Virgo Meeting, Stanford University, Palo Alto CA, August 24–29, 2014
- NARDA Meeting, California State University, Fullerton CA, August 21–22, 2014
- Gulf Coast Gravity Meeting, University of Mississippi, Oxford MS, April 19–20, 2013

2.3.3 Workshops and Summer Schools

- Extreme Gravity, Bozeman MT, August 20–22, 2015
- Observational Cosmology, ICTP-SAIFRSão Paulo, Brazil, December 1–12, 2014
- Testing General Relativity, University of Mississippi, Oxford MS, January 6–10, 2014
Chapter 3

Broader Impact

Since 2013, I have been actively participating in several seminar talks, schools, and workshops hold by IFT and ICTP-SAIFR. I also contributed directly yo ICTP-SAIFR scientific activities by delivering several technical talks in various occasions at ICTP-SAIFR including one on Gravitational Waves and Cosmology at the ICTP-Trieste/ICTP-SAIFR Workshop on Observational Cosmology in December 2014.

In November 2013, with Nicolás Bernal, another FAPESP fellow at ICTP-SAIFR, we started a biweekly Journal Club on Astrophysics and Cosmology at IFT-UNESP on Astrophysics and Cosmology (AC/JC). We successfully continued running this organized series of talks and discussion until this year. The participants are faculties, post-docs, and graduate students in the field of high energy physics from IFT-UNESP, ICTP-SAIFR, IAG-USP, and IF-USP. We also had several speakers from different institutes and universities from North America, Europe, and Asia. A website has been developed and continuously maintained at https://sites.google.com/site/ictpsaifrjc for a better organization and communication. This program that we started and organized is still running at ICTP-SAIFR. The new organizers are Fabio Iocco and Fabian Lacasa both from ICTP-SAIFR.

Working closely with Sturani, I put an strong effort on learning and developing new skills in Data Analysis and Machine Learning techniques in general, and Data Analysis of Gravitational Waves. I successfully achieved certificates of some high level online data analysis courses including Machine Learning and R programming offered by Stanford and Johns Hopkins Universities via Coursera. During 2014-2015, I also have gained valuable experiences on working with LAL code which is a massive collection of libraries and routines (in Python and C++ languages) to perform an accurate and comprehensive data analysis to be used as the main data analysis pipeline in advanced detectors such as Advanced LIGO.
Bibliography


Scientific Report

Non equilibrium First Principles molecular dynamics of solid/water interfaces: A novel approach to the study of electrochemical processes

Postdoc: Luana Sucupira Pedroza
Supervisor: Nathan Berkovits
FAPESP
Process: 2014/04114-3
31/12/14 to 31/03/15

ICTP-SAIFR / IFT-UNESP
São Paulo, SP
2015
1 Resumo do projeto

From a fundamental potion of view there is little understanding of the interactions at the liquid/solid interfaces. This is mostly due to the disordered nature of the liquid and the difficulty to properly describe it with empirical models. From a an application view, this understanding of the interaction of the water-solid system at an atomic level is extremely important in electrocatalysts for fuel cells, photocatalysis among other systems. To fully accomplish this task it is fundamental to describe all atoms and their interactions using first principles methodology, i.e., without empirical parameters.

However, in a more realistic system applied to catalysis, the metal will be charged. And an accurate calculation of the electrostatic potential at electrically biased metal-electrolyte interfaces is a current challenge for periodic \textit{ab initio} simulations. It is also an essential requisite for predicting the correspondence between the macroscopic voltage and the microscopic interfacial charge distribution in electrochemical fuel cells. This interfacial charge distribution is the result of the chemical bonding between solute and metal atoms, and therefore cannot be accurately calculated with the use of semi-empirical classical force fields. First principles methods, like Density Functional Theory (DFT) becomes then the most appropriate methodology.

We studied in detail the structure and dynamics of aqueous electrolytes at metallic interfaces taking into account the effect of the electrode potential. The electrode potential will be set by using the methodology already developed for the study of electronic transport in nano-structures. The \textit{ab initio} molecular dynamics (AIMD) simulations will be performed with the Siesta program, that is a code for electronic calculations based on DFT.

2 Atividades desenvolvidas

We proposed in this work to use open boundary conditions using the non-equilibrium Green’s function (NEGF) [1,2] method combined with DFT [3,4] to properly compute the effect of an external bias potential applied to electrodes. While standard DFT methods are not suited to treat extended systems under an external bias, NEGF has been designed to treat out-of-equilibrium situations. Their combination has been developed over the past few years to describe current-voltage characteristics of nanoscopic systems [2]. It treats an open system under the influence of an external bias, and albeit dynamics is typically ignored in such systems, it can be incorporated into the methodology. In this work, we apply this framework to a system consisting of a single water molecule on top of a Au(111) surface, at different configurations and as a function of an external voltage.

The equilibrium configuration for the water-metal system was obtained using the
Siesta code [5,6]. We have used two different gradient-dependent exchange-correlation (XC) functionals: PBE [7] and vdW-DF$^{PBE}$, the last one includes van der Waals corrections. The vdW-DF$^{PBE}$ is a modified version of the original vdW-DF functional [8], in which the revPBE local term was replaced by PBE. [9] The core electrons were described by norm-conserving pseudopotentials in the Troullier-Martins form. [10] A basis set of numerical atomic orbitals with double-$\zeta$ polarized (DZP) size were used to describe the valence electrons. For both metal and water the basis set was variationally optimized and ensured that our results (for Au lattice parameter, water-metal geometry) are in agreement with plane-wave calculations. All the atoms were allowed to move during the geometrical optimization, using the Conjugated Gradient algorithm and with a 0.005 eV/Å tolerance on the forces.

Our non-equilibrium calculations were performed using the Smeagol code [2] and the scattering region is defined as the metal-water-metal interfacial region. There, each metal slab has 3 layers of 12 Au atoms, with size $10.29 \times 9.89$ Å in the x-y plane. The water molecule is placed close to one metal surface (the one defined as left). In order to minimize the interaction between the surfaces, the right and left side are 20 Å apart. The electrodes, connected to the scattering region, consist of 3 Au layers each (left and right).

In order to analyze the effect of different bias (magnitude and sign) on the molecule as a function of the water orientation, we considered five different rigid rotations of the ground state configuration. For each configuration, we started at the ground state Au-O distance (2.79 Å, which corresponds to zero in the plots) and increased/decreased this distance from -0.5 to +2.0 Å and performed a single point calculation. At each point the force at the center of mass of the water molecule was evaluated as a function of the applied bias. The results are shown in Fig. 1 and Fig. 2.

In general, we observed that low bias (-0.5 and +0.5 V) has a small effect on the forces, independently of the water configuration. However, as we increase the applied bias we observe that the forces close to the minimum are modified. In particular, this effect is more evident for the flat molecule (Figs. 1) and for configurations where the oxygen is facing the metal, due to strong interaction between the $b_1$ orbital of the water molecule and the metal orbitals. [11]

In Fig. 1 it is possible to observe that there is a tendency to modify the position of the minimum configuration when the bias is applied. Moreover, this modification is dependent on the sign of the bias. The molecule tends to get closer to the metal when the bias is negative and oppositely it moves away from the metal with the positive bias. This behavior was also observed when vdW corrections are included, as shown in Fig. 3. In agreement to previous work [11], we note that the vdW functional does not change significantly the water-Au interaction. We note, however, that the barrier in all cases increases slightly for higher distances. This means that, although the equilibrium position of the molecule does not depend on the choice of XC functional,
Figure 1: Force at the center of mass as a function of the vertical displacement.

Figure 2: Force at the center of mass as a function of the vertical displacement for different water configurations.

the restoration force is larger when we include vdW interaction.
Figure 3: Force at the center of mass as a function of the vertical displacement for the flat water configuration, considering two different XC functional (PBE and vdW-DF$^{PBE}$).

3 Atividades acadêmicas

The results obtained during the postdoc were presented (oral presentation) at the 2015 APS March Meeting, in San Antonio, USA, entitled Bias-dependent local structure of water molecules at an electrochemical interface. At the moment, we are concluding the manuscript to be submitted to a journal with those results.

The week before the conference, I spent at Stony Brook University (NY, USA) working in collaboration with Prof. Marivi Fernandez-Serra. She is a co-author of this work and therefore it was very productive to stay there for discussions about the current work and future ones.

4 Atividades futuras

On November (2014) I was approved in the examination for an Adjunct Professor position at the Universidade Federal do ABC (UFABC). I started this position on 10th April 2015. Due this position, I concluded the postdoc earlier than the original plan (May 2016).
References


Scientific Report 2015

Title: Integrabilidade em teorias de gauge
Postdoc: Ryo Suzuki
Supervisor: Nathan Jacob Berkovits
Fapesp process: 2015/04030-7
Period: 01/10/2015 - 30/12/2015

INTERNATIONAL CENTER FOR THEORETICAL PHYSICS
SOUTH AMERICAN INSTITUTE FOR FUNDAMENTAL RESEARCH
Symmetry and dynamics have to be distinguished to understand physical models. The dynamics is difficult to predict, and one has to struggle with complicated calculation. The symmetry helps us simplify the problem, and makes us confident in our understanding. However, a model can have hidden symmetry, which is not obvious from the definition of the model.

Infinite-dimensional symmetry called integrability appears as hidden symmetry in many problems of gauge and string theories. The primary examples are the spectral problem of planar $\mathcal{N} = 4$ super Yang-Mills theory in 4-dimensions, and that of free superstring theory on $\text{AdS}_5 \times S^5$. According to a conjecture called AdS/CFT correspondence, both theories should describe exactly the same dynamics of strings on coincident D-branes. Physically, it is not obvious why this string-brane system possesses integrability. Mathematically, one can find that this system has the global superconformal symmetry $\mathfrak{psu}(2,2|4)$, part of which can be centrally-extended to the Yangian symmetry $Y(\mathfrak{su}(2|2)^2)$. The integrability (Yangian) helps us to demonstrate the AdS/CFT correspondence for the spectral problem.

The scheme of solving dynamical problems by finding and exploiting hidden symmetry of the theory should be generalizable in a broad range of examples. Below I describe specific problems and summarize my activities so far.

**Non-planar spectral problem.** In my last paper with Y. Kimura we found intriguing patterns in the non-planar operator mixing of planar zero modes (PZM) by numerical computation. Analytic computation was quite involved, which is generally true in non-planar problems.

A possible way to proceed further is to find a more sophisticated basis of operators. As the first step, we want to count the number of operators analytically as a function of length. Such a combinatorial problem is usually solved by applying Burnside’s lemma, or its generalization called Redfield’s formula. This formula correctly reproduces the number of all multi-trace operators and of PZM which are $\mathfrak{so}(6)$ singlets. To count the latter, it is important to consider permutation groups acting on pair sets. In physics language, we rewrite multi-trace operators as a set of flavor contractions, and the count all possible contractions; See Figure 1.

![](image.png)

**Figure 1:** Rewriting planar zero modes by flavor contraction operators.

**Four-point functions.** There is a resurge of interest in conformal bootstrap techniques, which allows us to compute four-point functions of general conformal field theories. In the AdS/CFT correspondence between $\mathcal{N} = 4$ super Yang-Mills and superstring on $\text{AdS}_5 \times S^5$, it is not well-understood how to apply the integrability methods to obtain non-perturbative four-point functions.

One of the obstacle is that the four-point functions are naturally related to non-planar corrections to the spectrum. The two data are related by the so-called extremal three-point functions, which is
responsible for the mixing between single-trace and multi-trace operators; See figure 2. I am trying to clarify the method to compute such three-point couplings.

\[
\mathcal{O}(1/N_c^2) = \mathcal{O}(1) \mathcal{O}(1) \mathcal{O}(1/N_c^2) + \mathcal{O}(1/N_c) \mathcal{O}(1/N_c) \mathcal{O}(1)
\]

Figure 2: Decomposing four-point functions into a two-point function and two three-point functions.

**Other academic activities.** Besides the research project, I have been organizing weekly journal club meetings for quantum field theory and string theory to enhance communication within the institute. I also take up a referee report.
FAPESP SCIENTIFIC REPORT
2015

Phenomenology of the
Large
Hadron Collider

Postdoc: Alberto Tonero
Supervisor: Nathan J. Berkovits
FAPESP
Process: 2013/02404-1
Period: 01/04/2013 to 30/12/2015

ICTP-SAIFR & IFT-UNESP
São Paulo
The first experimental run (2010-2013) of the Large Hadron Collider (LHC) has taken probes of the Standard Model of particle physics to an unprecedented level. The main result obtained by the experimental collaborations ATLAS and CMS was the discovery of a new boson with a mass of about 125 GeV. Even if the accumulated statistics was relatively low, a great effort has been made by the two main experimental collaborations in the attempt to define the properties of this new particle, namely its spin, parity and coupling constants to the particles of the Standard Model. These analyses point in favor of an Higgs boson as described by the Standard Model. This was a great triumph: the main block missing for the experimental validation of the Standard Model is now in place.

The second run of the Large Hadron Collider (LHC) has started in 2015 with a center of mass energy available in the proton-proton collisions that exceeds by an order of magnitude the previous collider experiments. The data coming from the new LHC run has started to be scrutinized by the experimental collaborations and this process will continue at least for the next five years when more data will be collected. The outcome of the analysis will either support the current Standard Model of particle physics with a fundamental scalar Higgs boson responsible for the breaking of the electroweak symmetry, or will indicate that there need to be important modifications of the Standard Model electroweak symmetry-breaking mechanism. Furthermore, the data may lead to clues for models beyond the Standard Model which include new features such as space-time supersymmetry or extra dimensions. Finally, the new data for high-energy ion collisions may shed light on properties of Quantum Chromodynamics such as confinement and the quark-gluon plasma.

The goal of the research project is to make use of the results obtained from the first LHC run together with the new data that are coming out from the second Large Hadron Collider run in order to interpret these measurements in light of theoretical models of particle physics.
During the year 2013 at ICTP-SAIFR I focused mainly my research activity on two projects related to particle physics phenomenology at the LHC.

The first project I have developed, together with two collaborators from SISSA (Italy), consisted in studying top quark compositeness using the most recent measurements coming from LHC and Tevatron. Whether the top quark is a point-like particle or an extended object is a question that can now be addressed thanks to the large number of them produced at the LHC and the Tevatron. If the top quark is a composite state made out of some constituents, its interaction with the gauge bosons will be modified. The most direct approach is to look into what effect a finite extension of the top quark has on its interaction with the gluon. In analogy with the study of the electromagnetic structure of nucleons, it is possible to parametrize effects of compositeness introducing two independent form factors modifying the vertex between the top quark and the gluon. These form factors can be used to obtain information about the radius and the anomalous magnetic moment of the top quark, in complete analogy with the nucleon case. Form factors are just a way of organizing the perturbative expansion. An alternative and perhaps better approach is effective field theory. In this study we introduced the leading effective operators that contribute to the radius and anomalous magnetic moment of the top quark and study their effect on the cross section for top-antitop production at the Tevatron and the LHC. The advantage of the effective theory approach is in the book-keeping because higher powers of the anomalous couplings enter suppressed by the higher dimension of the respective operators. We followed this latter approach and look only for solutions close to the standard model values. The most recent, combined measurement of the cross section for top-antitop production is in good agreement with the most up-to-date theoretical prediction within the standard model and this result can be used to put constraints on the compositeness of the top quark. Current measurements of the cross sections set a stringent limit on the scale of compositeness. This limit is comparable to similar limits obtained for light quarks and those from electroweak precision measurements. It can also be used to constrain the parameter space of many composite Higgs models. This work was presented in the E-print arXiv:1307.5750 [hep-ph] and was published in Phys.Rev. D89 (2014) 7, 074028.

The second project I started to work on together with R. Rosenfeld (IFT-UNESP) was about setting direct and indirect bounds on Standard Model dimension six operators, in particular the so-called 'dipole operators' involving the top-quark. These 'dipole operators' have direct effects on LHC observables because they give contributions to some physical observables that are going to be measured with an increasing precision in the next years. Preliminary LHC results about single top production cross section, W boson helicity fraction from top decay and top quark production in association to a weak vector boson are in agreement with the standard model predictions and these results can be used to put constraints on effective operators coefficients. I have performed a study about the effects of these dipole operators on these LHC observables. Using FeynRules and Madgraph 5, I have computed the contribution of these effective operators at linear order in the effective couplings to single top production cross section, W boson helicity fraction from top decay and top quark production in association to a Z and W vector boson. From these results I have derived 95% confidence level bounds on single operator coefficients. This work has been started in 2013 and was published in the following year.

During 2013 I started also to work with A. Codello and R. Percacci (SISSA) on a more theoretical project regarding the use of the Exact Renormalization Group Equation to compute the
effective action in quantum field theory. The Exact Renormalization Group Equation describes the functional renormalization group flow of the effective average action. The ordinary effective action is obtained by integrating the flow equation from an ultraviolet scale down to zero. The goal was to present several examples of such calculation at one-loop, both in renormalizable and in effective field theories. I was involved mainly in reproducing with this technique the four point scattering amplitude in scalar quantum field theories. I have studied in particular the case of a real scalar field theory with quartic potential and the case of the pion chiral lagrangian. We considered also gauge theories and we wanted to reproduce the vacuum polarization of QED and Yang Mills. The aim was to compute the two point functions for scalars and gravitons in the effective field theory of scalar fields minimally coupled to gravity.

Preprints and publications


Conferences and workshops

- "Workshop de Física César Natividade", 25-27 November 2013, Guaratinguetá (SP).

- “5th International Workshop High Energy Physics in the LHC era”, 16-20 December 2013, Valparaiso (Chile).

Visiting

I spent three weeks visiting ICTP Trieste in September 2013 under the agreement between the ICTP-SAIFR and ICTP Trieste. During that period I took the opportunity to work with my collaborators from SISSA in order to finalize the paper on top quark compositeness. Moreover I have started to develop the project about the application of the functional renormalization group equation to compute the effective action.
During the year 2014 my research activity at ICTP-SAIFR was focused mainly on two projects related to particle physics phenomenology at the LHC.

The first project I was involved in, together with two collaborators from SISSA (Italy), consisted in studying top quark anomalous couplings in the electro-weak sector using the most recent measurements coming from LHC and Tevatron. Currently available measurements from the Tevatron and the LHC already allow to set stringent limits on possible deviations in the values of these couplings from their Standard Model values. We reviewed and updated limits on possible anomalous couplings in the Wtb interaction vertex. Possible deviations in the interaction between the top quark and the neutral bosons Z and the photon were left out because still poorly measured. We consider data from top quark decay (as encoded in the W-boson helicity fractions) and single-top production (in the t-, s- and Wt-channels). We find improved limits with respect to previous results (in most cases of almost one order of magnitude) and extend the analysis to include four-quark contact interactions operators. We find that new electroweak physics is constrained to live above an energy scale between 430 GeV and 3.2 TeV, depending on the form of its contribution. This work was presented in the E-print arXiv:1406.5393 [hep-ph] and was published in Eur.Phys.J. C74 (2014) 12, 3193.

The second project I worked on, together with Rogerio Rosenfeld (IFT-UNESP), consisted in deriving direct bounds on the coefficients of higher dimensional top quark dipole operators from their contributions to anomalous top couplings that affect some related processes at the LHC. We assumed that the leading contributions to deviations from the Standard Model are encoded in the so-called top quark dipole operators and we present constraints on the coefficients of these operators arising from direct probes at the LHC. Several observables were studied. In our study we include the W helicity fractions in top quark decays, t-channel single top production, top pair production, associated tW production and, for the first time, top pair production in association with a vector boson. In this work we use the available LHC data for the processes listed above and we employ a Markov Chain Monte Carlo method to perform a Bayesian analysis in order to extract the posterior probability distributions for the coefficients of the dipole operators and the 1- and 2- sigma confidence level contours. This work was presented in the E-print arXiv:1404.2581 [hep-ph] and has been published in Phys.Rev. D90 (2014) 1, 017701.

In 2014 I have started, together with R. Rosenfeld (IFT-UNESP), a collaboration with Christoph Englert (Glasgow University) and Michael Spannowsky (Durham University) to work on a systematic investigation of the impact of beyond the Standard Model physics on Z boson pair and Z+Higgs production in the quark and gluon fusion channels using the language of effective field theory. We want to provide numerical codes as well as an in-depth investigation of all effective theory operators that are relevant for these analyses. These deliverables have been identified by the CERN Higgs cross section working group, and our results are guaranteed to have significant impact on ongoing and future analyses in this regard, especially given the close collaboration of the UK theory groups with the Glasgow ATLAS group.

Moreover, in collaboration with A. Codello (CP3-Origins, Odense), I have started to work on a new non-perturbative way to compute correlation functions in quantum field theories that account for the non-trivial renormalization group structure of the theory under consideration, using the Exact Renormalization Group Equation. The idea is to perform the path integral by weighting the momentum modes that contribute to it accordingly to their RG relevance, i.e. we weight a mode accordingly to the
value of the running coupling at that scale.

**Preprints and publications**


**Conferences and workshops**


- “Going On After the LHC8” workshop, 11-15 August 2014, ICTP-SAIFR, São Paulo, SP, Brazil.

- “XXXV Encontro Nacional de Física de Partículas e Campos”, 15-19 September 2014, Caxambu, MG, Brazil.

- “X SILAFAE”, 24-28 November 2014, Medellín, Colombia.
During the year 2015 I have finalized three projects related to LHC particle physics phenomenology and quantum field theory.

The first project I have completed in collaboration with A. Codello (CP3-Origins, Odense) was about a new non-perturbative way to compute correlation functions in quantum field theories that account for the non-trivial renormalization group structure of the theory under consideration, using the Exact Renormalization Group Equation. We have presented a simple and consistent way to compute correlation functions in interacting theories with non-trivial phase diagram. As an example we showed how to consistently compute the four-point function in three dimensional $\mathbb{Z}_2$–scalar theories. The idea was to perform the path integral by weighting the momentum modes that contribute to it according to their renormalization group (RG) relevance, i.e. we weight each mode according to the value of the running couplings at that scale. In this way, we are able encode in a loop computation the information regarding the RG trajectory along which we are integrating. We showed that depending on the initial condition, or initial point in the phase diagram, we obtain different behaviors of the four-point function at the end point of the flow. This work has been presented in the E-print arXiv:1504.00225 and has been accepted for publication in Phys.Rev. D.

The second project I have finalized during 2015 was the one related to the use of the Exact Renormalization Group Equation to compute the effective action in quantum field theory. The functional renormalization group is a way of studying the flow of infinitely many couplings as functions of an externally imposed cutoff. The idea originates from Wilson's understanding of the renormalization group as the change in the action that is necessary to obtain the same partition function when one flows towards the infrared starting from an ultraviolet cutoff. In particle physics one is usually more interested in the effective action than in the partition function, so one may anticipate that an equation describing the flow of the generator of one-particle irreducible Green functions may be of even greater use. For this purpose, the convenient functional to use is the effective average action. It is defined basically in the same way as the ordinary effective action, adding to the bare action a quadratic cutoff term. The effect of this term is to suppress the propagation of low momentum modes leaving the vertices unchanged. This equation has been widely used in studies of the infrared properties of statistical and particle physics models, in particular of phase transitions and critical phenomena. It has also been used to study the ultraviolet behavior of gravity, in particular to establish the existence of a nontrivial fixed point which may be used to define a continuum limit. In this project we discussed some examples taken from particle physics where the exact renormalization group equation is used instead as a tool to compute the effective action at one-loop. The ordinary effective action is obtained by integrating the flow equation from an ultraviolet scale down to zero. The goal was to present several examples of such calculation at one-loop, both in renormalizable and in effective field theories. I was involved mainly in reproducing with this technique the four point scattering amplitude in scalar quantum field theories. I have studied in particular the case of a real scalar field theory with quartic potential and the case of the pion chiral lagrangian. We have used the results of Barvinsky, Vilkovisky and Avramidi on the non-local heat kernel coefficients to reproduce the four point scattering amplitude in the case of a real scalar field theory with quartic potential and in the case of the pion chiral lagrangian. In the case of gauge theories, we have reproduced the vacuum polarization of QED and of Yang-Mills theory. We have also computed the two point functions for scalars and gravitons in the effective field theory of scalar fields minimally coupled to gravity. This work has been presented in the
The third project I have worked on in 2015 together with some collaborators from SISSA (Italy) was about $WW$ scattering at the LHC. Vector boson scattering (VBS) at the LHC provides a direct window on the mechanism responsible for the breaking of the electroweak (EW) symmetry. The tree-level amplitude for VBS is the combination of seven subprocesses in which gauge and Higgs bosons are exchanged. In the standard model (SM) the terms leading in energy cancel leaving an amplitude and a cross section consistent with unitary. If any or all among the trilinear and quartic gauge couplings and the Higgs boson coupling to the vector bosons are modified these delicate cancellations fail and tree-level unitarity is lost. In particular, if either the trilinear or the quartic gauge couplings are changed, terms proportional to the fourth power of the center-of-mass (CM) energy will be present. After the existence of the Higgs boson has been confirmed, we know that this particle plays a role in EW symmetry breaking but the details may differ from the basic scenario in which the Higgs boson is linearly and minimally coupled. If the gauge couplings are left unchanged but the Higgs boson couplings to the vector bosons are modified, terms proportional to the square of the CM energy will be present in the amplitude for VBS. All these potential departures from the SM represent signals for new physics. Since there are many possibilities, ranging from an extended Higgs sector to strong dynamics, they are best described by means of an effective field theory. In our work we have studied $W$ boson scattering in the same- and opposite-sign channels under the assumption that no resonances are present in the collider processes $pp \rightarrow l\nu l\nu jj$. Basic selection cuts together with a restriction on the combination of the final lepton and jet momenta (the Warsaw cut) makes it possible to argue that at the LHC a luminosity of 100 fb$^{-1}$ and a center-of-mass energy of 13 TeV will allow to constrain the leading effective lagrangian coefficients at the permil level. We also discuss limits on the other coefficients of the effective lagrangian as well as stronger constraints provided by higher energy and luminosity. We show that the same-sign $WW \rightarrow WW$ channel suffices in providing the most stringent constraints if coefficients are varied one at the time. This work has been presented in the E-print arXiv:1509.06378 and has been accepted for publication in *Phys.Rev. D*.

**Research plan**

I am including the description of future research projects since I am applying for a renewal of my fellowship in 2016.

I am currently working in collaboration with R. Rosenfeld (IFT-UNESP), Christoph Englert (Glasgow University) and Michael Spannowsky (Durham University) a systematic investigation of the impact of beyond the Standard Model physics on $Z$ boson pair and $Z+Higgs$ production in the quark and gluon fusion channels using the language of effective field theory. Motivated by interference effects observed and exploited in $gg \rightarrow ZZ$ production, we are investigating similar effects in the gluon fusion component of associated Higgs production $gg \rightarrow hZ$. It is known that the latter production mechanism can be relevant at the LHC in scenarios beyond the standard model, which can be constrained in boosted Higgs final states. Using a representative set of dimension-six operators, we provide an estimate of the sensitivity of such a search. Considering the full final state $gg \rightarrow bbl\ell^+\ell^-$, we discuss how the Higgs mass resolution in the boosted regime can influence the sensitivity yield as well as in how far new physics effects from $gg \rightarrow ZZ$ can leak into the $gg \rightarrow hZ$ signal region, thus decorrelating the sensitivity to BSM interactions. We aim to provide numerical codes as well as an in-depth investigation of all effective theory operators that are relevant for these analyses. These
deliverables have been identified by the CERN Higgs cross section working group, and our results are
guaranteed to have significant impact on ongoing and future analyses in this regard, especially given
the close collaboration of the UK theory groups with the Glasgow ATLAS group. This project is
supposed to be finalized by the beginning of 2016 and it will be submitted for publication.

I am also working together with S. Fichet (IFT-UNESP) and P. R. Teles (CMS, CERN) on a
project related to the optimization of shape analysis for effective operators at the LHC. Shape analysis
for effective operators is a powerful approach to look for new physics, and will be used in many
upcoming LHC analysis. This work is devoted to clarify and streamline the method of shape analysis
for effective operators, both technically and conceptually. We discuss the interplay between shape
analysis and EFT, and deduce the most economical exact method to carry out shape analysis. For a
given search and for n effective operators, we find that at most \((n + 1)(n + 2)/2\) points need to be
simulated in order to obtain the exact likelihood function. This likelihood function could then be used
as a basis for any hypothesis testing, like p-value based frequentist tests. However, we proceed by
observing that the Bayesian hypothesis test (i.e. the Bayes factor) can be computed either fully
analytically or through computationally light operations, for both real data and projected data.  This
work is supposed to be finalized by the beginning of 2016 and it will be submitted for publication.

In addition, I have started a project in collaboration with A. Codello (CP3-Origins, Odense)
about the heat-kernel computation of the RG flow of SM dimension-six operators. Dimension six
operators can have indirect effects on electroweak precision measurements as well as on Higgs
observables at the LHC, occurring through operator mixing. These effect can be studied computing the
renormalization group anomalous dimension mixing matrix. The standard way to perform this
computation is by means of Feynman diagrams which in this case can be quite involved due to large
number of them. An alternative approach we decided to follow consists in using heat-kernel techniques.
As a preliminary result, I have computed using heat kernel techniques loops of third generation quarks
which represent the renormalization group mixing matrix contributions to the pure bosonic operators
coming for dimension six operators of the fermion/boson mixed form. We want to extend the
preliminary heat kernel computation considering also bosonic and mixed loops my means of using
super heat kernel techniques, in order to obtain a full renormalization group mixing matrix.

Preprints and publications

- A. Codello and A. Tonero, “A renormalization group improved computation of correlation functions
  in theories with non-trivial phase diagram”, arXiv: 1504.00225 [hep-th], accepted for publication in
  Phys.Rev. D.

- A. Codello, R. Percacci, L. Rachwal and A. Tonero, “Computing the Effective Action with the
  Phys. Journ. C.

- M. Fabbrichesi, M. Pinamonti, A. Tonero and A. Urbano, “Vector boson scattering at the LHC. A
  study of the WW -> WW channels with the Warsaw cut”, arXiv:1509.06378 [hep-ph], accepted for
  publication in Phys.Rev. D.
Alberto Tonero

Conferences and workshops


- “XXXVI Encontro Nacional de Física de Partículas e Campos”, 14-18 September 2015, Caxambu, MG, Brazil.

- Workshop “Program on particle physics at the dawn of LHC13”, from October 19 to December 19 2015, ICTP-SAIFR, São Paulo, SP, Brazil.

Special seminars

- Colloquium at UFS “LHC physics and the Standard Model”, 23 September 2015, Aracaju, Sergipe, Brazil.

- Seminar “Vector boson scattering at the LHC. A study of the WW -> WW channels with the Warsaw cut”, 2 December 2015, USP São Carlos.

Visiting

I spent two weeks visiting the CERN Theory Group in June/July 2015 under the agreement between the ICTP-SAIFR and CERN Theory Group. During that period I took the opportunity to start working together with P. R. Teles (CMS, CERN) on the project related to the optimization of shape analysis for SM higher dimensional operators at the LHC.