## Scientific report for the period 31/12/2015 to 31/10/2016

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I joined the ICTP-SAIFR two years ago; my contract started on October  $1^{st}$  2013. The present report details my activities in 2016.

#### 1 Research

We consider scenarios where Dark Matter (DM) particles carry baryon and/or lepton numbers, which can be defined if there exist operators connecting the dark to the visible sector. As a result, the DM fields become intimately linked to the Standard Model (SM) ones and can be maximally asymmetric just like the ordinary matter. In particular, we discuss minimal scenarios where the DM is a complex scalar or a Dirac fermion coupled to operators with nonzero baryon and/or lepton numbers, and that consist of only SM fields. We consider an initial asymmetry stored in either the SM or the DM sector; the main role of these operators is to properly share the asymmetry between the two sectors, in accordance with observations. After the chemical decoupling, the DM and SM sectors do not care about each other as there is only an ineffective communication between them. Once the DM mass is specified, the Wilson coefficients of these operators are fixed by the requirement of the correct transfer of the asymmetry. We study the phenomenology of this framework at colliders, direct detection and indirect detection experiments. In particular, the LHC phenomenology is very rich and can be tested in different channels such as the two same-sign leptons with two jets, monojet and monojet with a monolepton (Ref. [1]).

DM halos have long been known to be triaxial, but in studies of possible annihilation and decay signals they are often treated as approximately spherical. In this work, we examine the asymmetry of potential indirect detection signals of DM annihilation and decay, exploiting the large statistics of the hydrodynamic simulation Illustris. We carefully investigate the effects of the baryons on the sphericity of annihilation and decay signals for both the case where the observer is at 8.5 kpc from the center of the halo (exemplified in the case of Milky Way-like halos), and for an observer situated well outside the halo. In the case of Galactic signals, we find that both annihilation and decay signals are expected to be quite symmetric, with axis ratios very different from 1 occurring rarely. In the case of extragalactic signals, while decay signals are still preferentially spherical, the axis ratio for annihilation signals has a much flatter distribution, with elongated profiles appearing frequently. Many of these elongated profiles are due to large subhalos and/or recent mergers. Comparing to gamma-ray emission from the Milky Way and X-ray maps of clusters, we find that the gamma-ray background appears less spherical/more elongated than the expected DM signal from the large majority of halos, and the Galactic gamma ray excess appears very spherical, while the X-ray data would be difficult to distinguish from a DM signal by elongation/sphericity measurements alone (Ref. [2]).

Collider, space, and Earth based experiments are now able to probe several extensions of the SM which provide viable DM candidates. It is remarkable that often the experiments that allow to reach the core region of the parameter space of several models -thus often ruling out sizable chunks of it- are either indirect, space based searches, or direct, earth based experiments. As it is well known, both types of experiments rely on inputs of astrophysical nature, such as e.g. the local DM density or the exact shape of the DM profile in the target. As it is equally well known, the determination of these quantities is affected by astrophysical uncertainties. The latter, especially those of our own Galaxy, are often ill–known, and not fully accounted for. We present a systematic, quantitative estimate of how astrophysical uncertainties on core Galactic quantities (such as the e.g. local galactocentric distance or circular velocity, or the morphology of the stellar disk and bulge) eventually propagate to the parameters of the particle physics model in case, thus affecting the determination of new physics. The results we obtain for two specific extensions of the SM, that we adopt as case studies, are extremely interesting, and show that a full account of the Galactic uncertainties is necessary when testing different regions of the particle-physic parameter space.

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.

#### 2 Publications

 Sharing but not Caring: Dark Matter and the Baryon Asymmetry of the Universe. Nicolás Bernal (ICTP - SAIFR), Chee Sheng Fong (Sao Paulo U.), Nayara Fonseca (Sao Paulo U. & DESY).

arXiv:1605.07188 [hep-ph], JCAP 1609 (2016) no.09, 005.

 Spherical Cows in Dark Matter Indirect Detection Nicolás Bernal (ICTP - SAIFR), Lina Necib, Tracy R. Slatyer (MIT, Cambridge, CTP). arXiv:1606.00433 [astro-ph.CO], submitted to JCAP.

#### 3 Seminars, Conferences & Workshops

#### 3.1 Seminars

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

- Mar. 4, 2016. 'WIMP and SIMP Dark Matter'. Universidade Cruzeiro do Sul, São Paulo, Brazil.
- 2. Apr. 14, 2016. 'The Dark Temperature'. ICTP-SAIFR, São Paulo, Brazil.
- May 9, 2016. 'Spherical Cows in Dark Matter Indirect Detection'. ICTP-SAIFR, São Paulo, Brazil.
- 4. Jun. 7, 2016. 'More on SIMP Dark Matter'. University of Warsaw, Warsaw, Poland.

- 5. Jul. 22, 2016. 'Spherical Cows in Dark Matter Indirect Detection'. HEPHY Institut für Hochenergiephysik, Vienna, Austria.
- 6. Sep. 29, 2016. 'Cannibal Dark Matter Yummy!'. ICTP-SAIFR, São Paulo, Brazil.

#### 3.2 Conferences and Workshops

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

- Jun. 2-5, 2016. Warsaw Workshop on Non-Standard Dark Matter: Multicomponent Scenarios and Beyond.
   'Z<sub>2</sub> SIMP Dark Matter'. Warsaw, Poland;
- Jul. 11-15, 2016. Xth International Conference on the Interconnection between Particle Physics and Cosmology (PPC).
   'SIMP Dark Matter'. ICTP-SAIFR, São Paulo, Brazil.

#### 3.3 Other Meetings

- Mar. 30 to Apr. 1, 2016. Dark Matter at the Large Hadron Collider 2016. Amsterdam, Netherlands.
- Jun. 27 to Jul. 9, 2016. School on Dark Matter. ICTP - SAIFR, São Paulo, Brazil.
- 11. Jun. 13-17, 2016. Bethe Forum on "Dark Matter Beyond Supersymmetry" Physikalisches Institut, Universität Bonn, Bonn, Germany.
- Oct. 25, 2016. III Dark Matter Day in São Paulo. ICTP - SAIFR, São Paulo, Brazil.

#### 4 Organization of Seminars

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

#### 4.1 Journal Club on Particle Phenomenology

Since the beginning of 2016, together with Alberto Tonero, we have been organizing the Journal Club on Particle Phenomenology. It has been scheduled weekly on Thursdays 2:00 pm in the room #3 of the IFT - UNESP.

#### 4.2 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, 29 webinars took place.

### 5 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
- Physical Letters B

## Research Report 2016

FAPESP REPORT PERIOD: AUGUST 2015- APRIL 2016

# Electronic properties and quantum transport in non-periodic systems

Dr. José Hugo Garcia Aguilar

supervised by Prof. Dr. Nathan BERKOVITS

April 15, 2016

### Introduction

One of the most direct probes of the electronic properties of materials is transport experiments. Where a sample is subjected to an external potential —usually an electric field— and the resultant current is measured. When this current is parallel to the applied field, one can relate its value to the band structure and density of state of the material[1]; moreover, when a transverse current is also measured, information about the topological structure of the electronic spectrum can also be obtained[2].

I specialize in calculation of the charge and spin conductivity tensor for disordered systems in the non-interacting regime. For this purpose, I use a real-space method developed by me and collaborators in 2015[3], which consist in using the kernel polynomial method[4] to approximate the Kubo-Bastin formula for the conductivity tensor[5] in terms of the Chebyshev polynomials basis.

During my time at ICTP-SAIFT, I applied this method in two types of non-periodic systems: graphene decorated with adatoms, in collaboration with Prof. Alexandre Rocha and Prof. Tatiana Rappoport and in quasicrystals, in collaboration with Prof. Eric Andrade. I have also developed a methodology based on genetic algorithm minimization[6, 7, 8] used to extract tight-binding parameters from ab-initio calculations. As a result of the research, I have submitted an article to a special issue of 2D Materials journal, and have other two in preparation. In the following I will show some results related to these works.

## 1 Spin-Hall effect in graphene by $sp_3$ hybridization

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[9]. These features make graphene a promising material for future electronics, and an interesting playground for fundamental research[9, 10, 11]. Due to the small value of its spin-orbit coupling and hyper-fine structure constant, graphene also has potential as a spin conductor; additionally, experimental evidence shows that doping graphene with other atoms such as hydrogen or copper [12, 13], could effectively enhance its spin-orbit coupling, allowing spin-current manipulation, which could open a way for graphene-based spintronic devices.

Different mechanisms are used to explain the enhancement of the spin-orbit coupling in graphene.  $sp_3$  hybridization [14, 15], hybridization with heavy adatoms [16, 17, 18] and proximity effects with cluster with large spin-orbit coupling[19, 20, 21]. In our work we focus decided to focus on  $sp_3$  hybridization mechanism, the main reason is that these type of mechanism seem to explain the enhancement measured in reference [12], and there are also recent theoretical predictions of other adatoms that could induce this type of enhancement in graphene[15]. However, in these proposes a direct connection to possible experimental measures such as the conductivity is still missing.

The starting point of our work is a model proposed by Gmitra at al[14] used to describe the adsorption of an atom at the T-site (above the carbon atom) of graphene. They use an Anderson Impurity model to describe the hybridization between the adatoms and graphene, and an additional term  $H_{\text{SOC}}$  describing the local spin-orbit coupling induced in graphene due to the hybridization. In their work the main conclusion is adsorption of adatoms at the *T*-site locally brakes the sub-lattice and out-of-plane mirror symmetry, allowing the existence of different spin-orbit terms, using density functional theory they found that in weakly hydrogenated graphene, only three different



Figure 1: Schematic representation of the local spin-orbit coupling due to adatoms adsorbed at the T-site (represented as blue). In panel (a) We show a local Rashba SOC interaction that connects the up and down spin sub-spaces. In panel (b) a local intrinsic-like interaction is shown, this interaction connects only sites with the same spin and it has a sign that depend of the neighbor being yellow for positive coupling and green the negative. In panel (c) We show the PIA interaction with connects next-nearest neighbor sites with different spins.

spin-orbit contributions are necessary:

$$H_{SOC} = H_R + H_I + H_{PIA} \tag{1.1}$$

where

$$H_R = \frac{2i\lambda_R}{3} \sum_{\langle i,j \rangle} c^{\dagger}_{i\sigma} c_{j\sigma'} \left[ \left( \hat{\boldsymbol{s}} \times \mathbf{d}_{ij} \right)_z \right]_{\sigma\sigma'}$$
(1.2)

is a Rashba-like interaction with coupling intensity  $\lambda_{\rm R}$ , where  $\hat{s} \equiv (s_x, s_y, s_z)$  is a vector of the  $s_x, s_y$ and  $s_z$  Pauli matrices, and  $d_i$  is a unitary vector connecting the adsorption site with its nearest neighbors with opposite spin as shown in Fig.1.(a), this term mixes the spin up and spin down sub-spaces breaking the  $s_z$  symmetry present in graphene.

$$H_I = \frac{i\lambda_I}{3\sqrt{3}} \sum_{\langle\langle i,j\rangle\rangle} c^{\dagger}_{i\sigma} c_{j\sigma'} \nu_{ij} [s_z]_{\sigma,\sigma'}$$
(1.3)

is a local intrinsic spin-orbit interaction with coupling intensity  $\lambda_{\rm I}$ , which couples the adsorption site with it next-nearest neighbors with the same spin, and  $\nu_{i,j} = \pm 1$  is a factor used to indicate and alternating sign between the six next-nearest neighbors as shown in Fig.1.b in green(positive sign) and yellow(negative sign). The third term is related to the  $C_{3v}$  symmetry that emerges when an adatom is adsorbed in the top position. It describes spin-flip hoppings between next-nearest neighbors:

$$H_{SOC} = \frac{2i\lambda_{\text{PIA}}}{3} \sum_{\langle\langle i,j\rangle\rangle} c^{\dagger}_{i\sigma} c_{j\sigma'} \Big[ \left( \hat{\boldsymbol{s}} \times \mathbf{D}_{ij} \right)_z \Big]_{\sigma\sigma'}.$$
 (1.4)

where  $\lambda_{\text{PIA}}$  is the strength of the novel SOC and D is a unitary vector conecting the next nearest neighbors with oposite spins as shown in Fig.1.c.

Our goal in this work was to understand the effect of  $H_{\text{SOC}}$  in spin transport measurement as a function of coupling intensity and concentration of adatoms. The main conclusion is that although  $H_{\text{SOC}}$  can be decomposed into three contribution only the Rashba-like and the Intrinsiclike contribute to spin-transport in the low concentration and weak coupling limit. We also showed there is basically no effect into the charge transport due to the Intrinsic contribution while Rashba and the pseudo-spin inversion asymmetry seem to create localized states outside the Fermi Energy.

#### 1.1 Results

We performed a systematic analysis of each term by individually as a function of concentration and coupling intensity. We performed our calculations in a honeycomb lattice with  $D = 2 \times 200 \times 200$  sites with a dilution ranging from 5% - 40% and couplings ranging from 0.1t - 0.4t, using a Chebyshev expansion truncated at M = 800 for the conductivity tensor and density of state calculations.

#### 1.1.1 Rashba Interaction

Our first analysis is for a distribution of pure Rashba spin-orbit impurities ( $\lambda_I = \lambda_{PIA} = 0$ ) as a function of intensity of the coupling can be seen in Fig.2, where we keep the concentration fixed (x = 0.2). In the density of states shown in Fig.2.c, we notice the presence of new states at the neutrality point. These states are extended as can be seen in panel 2.a with an slight increase in the minimum of the longitudinal conductivity for increasing values of the spin-orbit coupling. At the same time, the Rashba coupling strongly suppress the longitudinal conductivity away from the charge neutrality point. The spin Hall conductivity changes signs with the energy and it is zero at the Dirac point, as expected (see Fig.2.c). However in the vicinity of the E = 0 there is a rapid increase of the spin Hall conductivity that saturates at  $\approx \pm e/(2\pi)$ , which is consistent with analytical calculations for the SHE in graphene with constant RSO[22]. The transition from negative to positive spin Hall conductivity as a function of the chemical potential gets more abrupt for weak  $\lambda_R$ . Surprisingly, this translates into an *increase* of the spin Hall effect in the vicinity of the neutrality point for *decreasing* values of  $\lambda_R$ , as shown in Fig.2.d.



Figure 2: Graphene decorated with a random distribution of RSO-impurities ( $\lambda_I = \lambda_{PIA} = 0$ ) sitting at the *T*-site.  $D = 2 \times 200 \times 200$  sites, concentration of x = 0.2 and M = 800. (a) Longitudinal conductivity and (b) spin Hall conductivity as a function of the chemical potential for increasing values of the intensity of the ISO coupling. (c) Density of state (d) Spin Hall conductivity as a function of the spin-orbit intensity for different values of the Fermi energy: (Black) 0.05t, (Red) 0.1t, (Blue) 0.5t.

In Fig.3 we show the results as a function of the concentration, fixing the RSO coupling in  $\lambda_{RSO} = 0.4t$ . Again, the system becomes progressively more metallic for increasing concentration in the low energy limit (see Fig.3.b). The dependence of the spin Hall conductivity with concentration is shown in Fig.3.c, where we see a rapid increase in the spin Hall conductivity.

the Dirac point when the concentration is reduced. Furthermore, Fig.3.d indicates a dependency of 1/x for the spin Hall conductivity at a fixed chemical potential close to the neutrality point up to x = 0.05. Lower concentrations of impurities, not accessible in our analysis, may affect the spin Hall effect in a different way. Our results indicate that Rashba tends to delocalize the electrons, inducing a metallic behavior near the Dirac point. Additionally, they suggest that the spin Hall conductivity generated by Rashba must be relevant in experiments: it is larger for low concentrations and weak Rashba spin-orbit coupling, as it is expected for graphene with adatoms.



Figure 3: Graphene decorated with a random distribution of RSO-impurities ( $\lambda_I = \lambda_{PIA} = 0$ ) sitting at the *T*-site.  $D = 2 \times 200 \times 200$  sites,  $\lambda_R = 0.4t$  and M = 800. (a) Longitudinal conductivity and (b) spin Hall conductivity as a function of the chemical potential for increasing values of concentration *x*. (c) Density of state (d) Spin Hall conductivity as a function of the concentration for different values of the chemical potential: (Black) 0.05t, (Red) 0.1t, (Blue) 0.5t.

#### **1.2** Intrinsec Interaction

Next we consider the effect of  $H_I$ . In Fig.4 we show the KPM numerical calculations with M = 1600 moments for a honeycomb lattice decorated with a random distribution of pure intrinsic adatoms  $(\lambda_R = \lambda_{PIA} = 0)$ . The density of states is shown in Fig.4.c where the presence of a band gap is observed. This gap translates into a region of zero longitudinal conductivity, shown in Fig.4.b.

For this concentration, the value of the gap follows the following relation

$$\Delta_{ISO} \propto x \lambda_I,$$

which is consistent with Kane and Mele [23] model rescaled by the concentration and agrees with previous numerical calculations [24, 3]. For intensities below  $\lambda_I = 0.1t$ , the gaps close due to the effect of the temperature.



Figure 4: Graphene decorated with a random distribution of ISO-impurities ( $\lambda_R = \lambda_{PIA} = 0$ ) sitting at the *T*-site.  $D = 2 \times 200 \times 200$  sites, concentration of x = 0.2 and M = 1600. (a) Longitudinal conductivity (b) Spin Hall conductivity as a function of the chemical potential for increasing values of the intensity of the ISO coupling. (c) Density of state (d) Spin Hall conductivity as a function of the spin-orbit intensity for different values of the Fermi energy: (Black) 0.02t, (Red) 0.05t, (Blue) 0.1t.

In Fig.5.c we can see that inside the gap, the system presents quantized spin Hall conductivity as expected from the Kane and Mele model. However, we observe that outside the gapped region a robust spin Hall conductivity still persists, a fact that can be important in experiments where the strength of the ISO coupling is usually small and the gap is closed.



Figure 5: Graphene decorated with a random distribution of ISO-impurities ( $\lambda_R = \lambda_{PIA} = 0$ ) sitting at the *T*-site.  $D = 2 \times 200 \times 200$  sites,  $\lambda_I = 0.4t$  and M = 1600. (a) Longitudinal conductivity (b) Spin Hall conductivity as a function of the chemical potential for increasing values of the concentration *x*. (c) Density of state (d) Spin Hall conductivity as a function of the concentration for different values of the Fermi energy: (Black) 0.02t, (Red) 0.05t, (Blue) 0.1t.

#### 1.3 Pseudo-spin Inversion Assymetry (PIA) interaction

Fig. 6 presents the results for the pure PIA impurities ( $\lambda_I = \lambda_R = 0$ ) for increasing spin-orbit coupling with x = 0.2 and M = 800. In the density of states, shown in Fig.6.c, we can see the emergence of new states in the vicinity of the Dirac point. These new states are more localized, as can be seen in Fig.6.a, where a reduction in the electronic mobility is detected. Fig.6.c, displays the spin Hall conductivity that saturates at high energies with a saturation value that depends directly on the coupling intensity. In Fig.6.d we show the behavior of the spin Hall conductivity in the vicinity of the neutrality point. In contrast with the RSO, for PIA, the spin Hall conductivity increases with the coupling strength and it is small (tending to zero) in the low coupling regime.



Figure 6: Graphene decorated with a random distribution of PIA-impurities ( $\lambda_I = \lambda_R = 0$ ) sitting at the *T*-site.  $D = 2 \times 200 \times 200$  sites, concentration of x = 0.2 and M = 800. (a) Longitudinal conductivity and (b) spin Hall conductivity as a function of the chemical potential for increasing values of the intensity of the ISO coupling. (c) Density of state (d) Spin Hall conductivity as a function of the spin-orbit intensity for different values of the Fermi energy: (Black) 0.02t, (Red) 0.05t, (Blue) 0.1t.

Finally, we consider  $\lambda_{PIA} = 0.4t$  and display the results as a function of the concentration x (Fig.7). In the density of states shown in Fig.7.c, we can see again the presence of new localized states in the vicinity of the Fermi energy, which is confirmed by a decrease in the longitudinal conductivity (see Fig.7.a). In Fig.7.c one can see that the spin Hall conductivity quickly saturates at high energy as a function of the concentration. Near the neutrality point, the behavior is shown in Fig.7.d, where the spin Hall conductivity increases with concentration and tends to zero for small concentrations. Our results show that PIA induces new localized states in the vicinity of the neutrality point. They also indicate that the spin Hall effect induced by PIA must be negligible under realistic experimental conditions were the SOC is weak and the concentrations are small.

#### 1.4 Conclusions

For the intrinsic spin-orbit coupling, where the appearance of a quantum spin Hall state is expected, we observed a linear dependence of the size of the gap with the concentration of adatoms, for all cases considered here. We also showed the presence of robust spin Hall conductivity outside the topological gap. We found that Rashba induces robust spin Hall conductivity for low concentrations and weak coupling which is an important limit to compare with experimental results.



Figure 7: Graphene decorated with a random distribution of PIA-impurities ( $\lambda_I = \lambda_{PIA} = 0$ ) sitting at the *T*-site.  $D = 2 \times 200 \times 200$  sites,  $\lambda_P IA = 0.4t$  and M = 800. (a) The longitudinal conductivity and (b) spin Hall conductivity as a function of the chemical potential for increasing values of concentration *x*. (c) Density of state (d) Spin Hall conductivity as a function of the concentration for different values of the chemical potential: (Black) 0.02t, (Red) 0.05t, (Blue) 0.1t.

Conversely, PIA tends to localize electrons and does not contribute to the spin Hall conductivity in the low concentration and weak coupling limit. In conclusion, both intrinsic and Rashba spin-orbit couplings should be relevant in the regime of parameters that are typically found in experiments. Furthermore, even at finite temperatures and in the presence of disorder, they can give rise to non-quantized but sizable spin Hall conductivities.

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# 2 Assymetric spin-orbit coupling in Graphene due to hidroxide adsortion

In the previous section we presented a first work where we study the effect on spin-current due to  $sp_3$  hybridization. However, we used a model derived for hydrogen adsorption[14] and later used on Fluor[15]; however, in both systems there is a well-defined spherically symmetric s orbital. Which lead to a symmetric model for the hybridization and of the  $H_{SOC}$  term. The simplest variant to this model would be to consider another atom that also creates a  $sp_3$  hybridization, but with an additional degree of freedom to include an asymmetry to the system in order to study the effect of breaking the rotational symmetry of graphene. We choose hydroxide molecule for this purpose,



Figure 8: (a) The relaxed structured obtained from the ab-initio calculation showing that hydroxide is adsorbed on top of a carbon atom, and that it also creates the pyramidal structure which characterise the  $sp_3$  hybridisation.

because it possess this two features, and in this work in progress we explore the possibility of an asymmetric spin-orbit coupling in graphene. In a first step, we calculate the electronic band structure of hydroxide adsorbed in a  $5 \times 5$  graphene super cell relaxed until the total force is less than 0.005 eV/Ang. This calculation were performed using the SIESTA code [25, 26] using numerical atomic orbitals with double zeta polarization (DZP) basis set with confinement energy of 0.001 Ry and a  $16 \times 16 \times 1$  Monkhorst-Pack of k points was used for sampling Brillouin zone. For the core we used improved Troullier Martin, norm conserving, relativistic pseudopotentials[27] for both carbon, hydrogen and oxygen and the exchange and correlation energies are treated within the local density approximation according to the Ceperlay Alder parameterization[28].



Figure 9: The electronic bands structure of hydroxide adsorbed at the center of a  $5 \times 5$  graphene's super cell. In solid line we present the result obtained from DFT calculation in black is the conduction band, in red the mid-gap states due to the hydroxide molecule and in blue the valence bands. In dashed lines we present our fit obtained through the simplified model in Eq.2.2

In Fig.8 one can see that hydroxide is adsorbed at the T-site just like Hydrogen, and it creates a a pyramidal local deformation in graphene's plane increasing the carbon bond length in 1%, which is similar to what happen with hydrogen; however, in this case there is also an asymmetry due to the angle formed by the vertical and the oxygen-carbon bond which is roughly 10. In Fig.9 we show the band structures in solid lines, the gap in the band structure is due to the periodicity

of the impurity; nonetheless the three bands present near the Fermi level, should be still relevant when considered a distribution of impurities. In order to see if the asymmetry present in the relaxed structure has any effect on the electronic properties, we looked at the two-dimension charge distribution at graphene's plane defined as:

$$\sigma_l(x,y) = \int_{z_-}^{z_+} \int_{\varepsilon_-}^{\varepsilon_+} \rho(x,y,z,\varepsilon) d\varepsilon dz$$
(2.1)

where the range  $z \in [z_-, z_+]$  is computed to include graphene and the impurity and the range  $\varepsilon \in [\varepsilon_-, \varepsilon_+]$  are the range of energy of the electrons we are considering, in this case we choose this range in order to include the electrons belonging to the three bands in Fig.9. The result is shown in Fig.10.(a) where we see there is a slight asymmetry distribution for the states near the adsorption site.



Figure 10: (a) The relaxed structured obtained from the ab-initio calculation showing that hydroxide is adsorbed on top of a carbon atom, and that it also creates the pyramidal structure which characterize  $sp_3$  hybridization. (b). Local Density of states for the relaxed system projected in the xy-plane of graphene, asymmetry of 1%

#### 2.1 The model

In order to perform large scale transport calculations such as the performed in Section 1, it is desirable to construct a simplified tight-binding model describing the adsorption of hydroxide. In order to construct the model we started we a general tight-binding Hamiltonian for the hybridization part

$$H_{\rm hyb} = H_0 + \varepsilon_I c_I c_I + \sum_{\langle I,i \rangle} \varepsilon_i c_i^{\dagger} c_i + \sum_{\langle I,i \rangle} \left( \tau_{I,i} c_I^{\dagger} c_i + h.c \right)$$
(2.2)

where  $H_0$  is pristine graphene Hamiltonian, and the hydroxide effect is modeled considering a change in the on-site energy at the adsorption site  $\varepsilon_I$ , a change in the on-site energies  $\{\varepsilon_i\}$  at the nearest neighbors of the adsorption site, and a change in the hopping parameters  $\{\tau_{I,i}\}$  connecting the adsorption site with its nearest-neighbors. Therefore, the model has seven parameters to fit initially. We used a genetic-algorithm minimization procedure in order to find a reduced number of parameter and to fit them simultaneously. In this procedures a random set of solution is created initially and it is then mixed in order to satisfy a given minimization criteria, in this case leastsquares and the maximum number of parameters. This procedure is very general and can be used for any system and any type of minimization. The genetic algorithm minimization was performed using our implementation using a set of 50 initial solutions, mixed in a pool of 300 offspring, we used non-linear ranking and universal sampling to choose the better solutions and in each iteration 50% of the population is discarded. The genetic algorithm generated a a model with only three parameters showed in the Fig.10.(b). The band structure for this model is shown in dashed lines in Fig.9, and one can see this model describe well the band structure and specially it can describe very well the K and K' points which are the most important for transport measurements.

#### 2.2 Work in progress

In the current state of this work we performed DFT calculations including spin-orbit effect. The bands splitting are shown in Fig. 11



Figure 11: Difference between spin-up and spin-down conduction(black), midgap(red) and valence(blue) bands of hydroxide adsorbed at the center of a  $5 \times 5$  grapehene's supercell.

the spin-splitting profile is very similar to the obtained in previous work for symmetric adatoms [14, 15], except of the discontinuities at the Dirac points, we are now using the genetic algorithm procedure to generate a spin-orbit model to see if there is any connection between these features and the asymmetries observed above.

### 3 Quasicrystals

Another important non-periodic system is quasicrystals, where the atoms organize themselves into a highly-ordered structure which is nevertheless entirely aperiodic. 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[29]. However, when these approximants are small, they are more metallic than quasicrystals and don't accurately reproduce many features related to the lack of periodicity such as criticality, and fractality of the wave function[29].



Figure 12: (a) The density of states calculated for an approximant of 68000 sites. (b) Comparison Between the density of states and the typical density of states for the same approximant. (c) Distribution of local density of states for different energies

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[30, 31]. 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 whether the electronic wave function of the system is localized or extended[30, 31]. Within this approach one can also obtain information about the fractality of the wave function and the criticality of the system [32], all can be measured experimentally [33].

In Fig. 12, we have the preliminary results for these calculations. We show the density of states of an approximant with ~  $10^5$  sites , and it agrees perfectly with others found in the literature[34, 35]. 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 thant the states at the boundary. Finally we compute the probability distribution function to see its it behavior is similar to the one expected for metals at the cristical 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.

### 4 Publication during 2015-2016

 Jose H. Garcia, Tatiana G. Rappoport, Kubo-Bastin approach for the spin Hall conductivity of decorated graphene, arXiv:1602.04864. Submitted to 2D Materials, ref. num. 2DM-100422.R.

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# **Scientific report**

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

Postdoc : Chrysostomos Kalousios Supervisor : Nathan Jacob Berkovits FAPESP Process: 2012/00756-5 Period: 1/10/2015 to 30/9/2016

XRY Math Blo

### Scientific report for the period 1/10/2015 to 30/9/2016

Chrysostomos Kalousios

#### Personal Information

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#### Service and Outreach

Referee for JHEP.

#### Invited talks, Presentations and Workshops

Participant in "School on Fundamental Aspects of String Theory", ICTP, São Paulo, Brazil, May 23-30, 2016.

Participant in "VIII Workshop on String Field Theory and Related Aspects", ICTP, São Paulo, Brazil, May 31-June 3, 2016.

Invited talk, University of Southampton, United Kingdom, June 15, 2016.

Participant in "Journeys into Theoretical Physics", ICTP, São Paulo, Brazil, July 18-23, 2016.

Invited talk, Universidad Andrés Bello, Santiago, Chile, September 21, 2016.

Participant in "Workshop on 3-point functions in Gauge/String theories", ICTP, São Paulo, Brazil, September 19-30, 2016.

- C. Cardona and C. Kalousios, "Comments on the evaluation of massless scattering". JHEP 1601, 178 (2016). arXiv:1509.08908 [hep-th].
- C. Cardona and C. Kalousios, "Elimination and recursions in the scattering equations". Phys. Lett. B 756, 180 (2016). arXiv:1511.05915 [hep-th].
- C. Kalousios, "Getting compact expressions in massless scattering" (in preparation).

### Published

#### Comments on the evaluation of massless scattering [1]

In this work Carlos Cardona and I 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 [2] 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 [3] and an algorithm presented by one of the authors in [2]. 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 [2], where the coefficients of polynomials where put in use through the well-known in mathematics Vieta formulas.

#### Elimination and recursions in the scattering equations [4]

In this work Carlos Cardona and I examine the problem of finding solutions of the scattering equations. This is an important problem, because knowledge of the solutions of the scattering equations is directly associated to the evaluation of the scattering amplitude. We use the elimination theory to express all variables of the scattering equations in terms of one variable. Then we construct the polynomial equations that the last variable of the scattering equations satisfies. We give two different but equivalent methods to achieve this. The first one is based on the Sylvester method and the second one on the Bezout method.

### In preparation

#### Getting compact expressions in massless scattering

This work is mostly finished, but not yet submitted for publication. It is related to the evaluation of scattering of massless particles using the scattering equations. In this work I observe that one does not need to know the explicit solutions of the scattering equations in order to evaluate the amplitudes. One can use the elimination theory from mathematics in a specific way that allows the extraction of all the useful information. Moreover, the resulted expressions are given directly in a compact form in terms of determinants. This allows us to express lengthy scattering amplitude expressions in an organized way. Furthermore, new unknown expression are evaluated for general number of external particles.

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## Scientific report 2016

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 : 1/1/2016 - 31/7/2016

not School

ICTP-SAIFR Sao Paulo

## Scientific report 2016

#### Fabien Lacasa

This report is additional to the 2015 scientific report which describes my work at ICTP-SAIFR from December 1st 2013 until December 31st 2015. It is supposed to be read with that previous report in mind, and implicitly refers to it several times. The present report describes additional activities which occured from January 1st 2016 to July 31st 2016.

During that period I kept my involvement in the *Planck* and *Dark Energy Survey* collaborations, as well as co-supervising undergraduate student Nickolas Kokron (bolsa FAPESP de Iniciação Científica) together with Prof. Rogerio Rosenfeld.

### **1** Presentations

#### 1.1 Seminars

- March 4th 2016 at Institut d'Astrophysique Spatiale (Orsay, France) : Dark Energy Survey

- April 14th at Instituto de Astronomia e Geologia (USP, São Paulo) : Combined cosmological probes : cluster abundances and galaxy clustering

- May 17th at Laboratoire de l'Accélérateur Linéaire (Orsay, France) : Combined cosmological probes : cluster abundances and galaxy clustering

- June 17th at DES-Brazil Science Day (webinar between ICTP-SAIFR, IF USP and Observatorio Nacional de Rio) : Combined cosmological probes : cluster abundances and galaxy clustering

### 2 Publications

This pdf hyperlink<sup>1</sup> should get you to a list of most of my publications on the NASA Astrophysics Data System (ADS). This other pdf hyperlink<sup>2</sup> gets you to my publication list on inSPIRE, which is a bit more complete.

With Prof. Rogerio Rosenfeld we submitted in April the following article to the Journal of Cosmology and Astroparticle  $Physics^3$ :

- Combining cluster number counts and galaxy clustering arXiv:1603.00918, ADS link<sup>4</sup> we received a positive referee report mid-June and are currently answering the referee's comments for final acceptance.

### 3 Supervision

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

<sup>&</sup>lt;sup>1</sup>http://adsabs.harvard.edu/cgi-bin/nph-abs\_connect?arxiv\_sel=astro-ph&author=Lacasa%2C+F.

 $<sup>^{2} \</sup>tt http://inspirehep.net/search?p=exact author\% 3AF.Lacasa.1\&sf=earliest date$ 

<sup>&</sup>lt;sup>3</sup>http://iopscience.iop.org/journal/1475-7516;jsessionid=701A349F095A4D701DC48A41674D46E1.c1. iopscience.cld.iop.org

<sup>&</sup>lt;sup>4</sup>http://adsabs.harvard.edu/abs/2016arXiv160300918L

#### 4 Research statement

#### 4.1 in Dark Energy Survey (DES)

I worked with Prof. Rogerio Rosenfeld on combining cluster number counts and galaxy clustering, which lead to the article presented in Section 2. We have indeed studied theoretically the prospect of combining the information of these two important cosmological probes, which are going to be studied in DES. Both these probes are sensitive to the large scale structure of the universe, which produces two effects :

- some of their separate information content is common/redundant

- their error bars are correlated

the latter point may easily be overlooked by physicists from another domain than cosmology, where measurement errors have a different origin than the signal. However cosmological observables are intrinsically stochastic and as such measurements can be limited simply by the sampling variance, also known as cosmic variance.

It has indeed be the goal of this project to predict theoretically this cosmic variance for these two probes and their correlation : their covariance. To this end one requires a non-linear description of the large scale structure of the universe. We have been using the halo model combined with a Halo Occupation Distribution, and have shown that a non-perturbatively non-linear model is indeed required for realistic predictions.

Additionally to these theoretical predictions, I have been collaborating with Kai Hoffmann and Enrique Gaztañaga (ICE Barcelona) in order to measure cluster counts, the galaxy power spectrum and their covariances in the MICE<sup>5</sup> simulations. Progresses were made both on the measurement and prediction side, in particular through collaboration with Michel Aguena and Marcos Lima (IF USP) that allowed me to produce reliable super-sample covariance predictions in the case of partial sky coverage. We are now reaching convergence between measurements and predictions, which will allow us to study next the dependence of the covariances on redshift and sample selection (e.g. magnitude or color cuts). We should be writing an article presenting our findings in the coming months.

A second part of my work was devoted more importantly to DES data analysis and characterization, in particular within the Large Scale Structure (LSS) working group. In particular with graduate student Nickolas Kokron (see Sect. 3), we have been developing the measurement of the galaxy angular power spectrum for the coming analysis of the Baryonic Acoustic Oscillations (BAO) in DES first year data. We have been developing the methodology for this measurement, gone for extensive validation on simulations (both homemade and with the aforementionned MICE), compared with measurement by other DES groups, and performed the actual measurement on all DES catalogue candidates to date. In collaboration with Flavia Sobreira (UFABC, Santo André), we are currently developing the pipeline for the cosmological interpretation of the measurement : the BAO detection and characterization. These works should be part of the official DES first year results, to be published later this year, which I think is a very nice results for an undergraduate project.

Furthermore, I have been collaborating on several DES-Brazil activities, as a support on questions of statistics, halo model, power spectrum and Halo Occupation Distribution (HOD). And I am currently getting involved in new DES projects : analysis of the cluster clustering, and of the galaxy 3-point function.

#### 4.2 Others

I have also been working in collaboration with other scientists abroad, particularly in Europe.

First, I have kept working on a model of the bispectrum of the Cosmic Infrared Background (CIB) anisotropies, together with Aurélie Pénin (UKZN, South Africa) and Stéphane Ilic (CPT Marseille, France). We have indeed developed a model which accounts for all the latest progresses in the

<sup>&</sup>lt;sup>5</sup>http://maia.ice.cat/mice

understanding of the CIB physics, in order to interpret the Planck measurements. Results are now finalized and we are currently writing teh article describing them, article which should be submitted for publication later this year.

Then I have also kept on working on the modelisation of the bispectrum of the thermal Sunyaev-Zel'dovich (tSZ) effect, in collaboration with Guillaume Hurier (CEFCA, Spain), Mariand Douspis and Nabila Aghanim (Institut d'Astrophysique Spatiale, Orsay). Redaction of the results was delayed by personnal circumstances in the group and needs to be resumed. However, we have been finding that cosmological constraints from the tSZ bispectrum are competitive with, if not better than, that from the power spectrum, an interesting and exciting result. Several spin-off projects have been discussed for the future, particularly in relation with the coming Euclid data (mission to be launched in 2020).

Furthermore, I launched a new project in collaboration with Agnès Ferté (University of Edimbourgh, Scotland) and Julien Grain (Institut d'Astrophysique Spatiale, Orsay France). We aim to develop for galaxy gravitational lensing, the use of data nalysis methods originally aimed for polarization of the Comic Microwave Background. Indeed both observables are spin-2 fields on the celestial sphere and are thus characterized by their E and B modes, whose estimation is hindered by leakage in the partial sky case. So-called purification methods are aimed at reducing, if not cancelling, this leakage, which is particularly important if one wants to detect the trace of beyond the standard model physics in the subleading B modes. And such motivation is indeed present following recently published articles on the possibility to test the isotropy of the expansion of the universe with weak-lensing observables, in particular the mentioned B modes. To test these ideas, we are developing collaboration with their promoters namely Jean-Philippe Uzan, Cyril Pitrou (Institut d'Astrophysique de Paris, France) and Thiago S. Pereira (Universidade Estadual de Londrina, Paraná Brazil).

Finally, and in preparation for my future postdoc there, I have been invited to the University of Geneva, where I have discussed and launched new projects with Martin Kunz, Ruth Dürrer (Université de Genève, Switzerland), Julian Adamek (Observatoire de Paris-Meudon, France) and Julien Carron (University of Sussex, United Kingdom). Specifically these are projects aimed at extracting the additional non-Gaussian information from observables of the large scale structure of the universe, as well as detecting non-linear effects of General Relativity (or modified gravity theories) beyond the, until now sufficient, newtonian approximation. These projects will particularly be pertinent for the coming Euclid mission, in which I am getting involved.

# FAPESP SCIENTIFIC REPORT 2016

# Coalescence of Binary Systems with Eccentricity

Postdoc : Alessandro Parisi Supervisor : Nathan J. Berkovits Process : 2016/00096-6 Period : 01/04/2016 to 30/11/2016

> ICTP-SAIFR & IFT-UNESP Sãn Paulo

Dessanches Parisi Natt Bulat

# Resumo do projeto

This project aims at maximising the scientific exploitation of GW through advancements beyond current state of the art in rapid automated analyses, background discrimination, and waveform reconstruction.

The aim of my project is to investigate the possibility that eccentricity leads to a deformation that can excite the mode f of the star, which in turn generate their own characteristic GW signal. The heart of my project is to understand whether f-mode oscillation give a significantly contribute to the gravitational wave emission during the "inspiral" phase of the system.

The implementations of the Einstein equations, relativistic hydrodynamics equations allowus to test any realistic EoS which describe both nuclear matter and quark matter, then the sensitive dependence of the binary evolution on orbital parameters, signals from orbit induced stellar oscillations can give constraints for a more realistic EoS, including a quantification of the shock heating and the possibility of the formation of a hyper-massive compact star.

My current projects include: understanding the nature of binary compact objects (black hole and compact star) during the inspiral phase, the stability and dynamics of these objects.

The non-linearity and complexity of Einstein's equations make it challenging to solve even numerically, also the evolution of the system is strongly dependent on the initial data for fully relativistic simulations is a very delicate task. My study does not intend to be exhaustive, since many more equations of state may be considered in the analysis and also deviations from the adiabatic evolution are difficult to include.

I also intend to explore the detectability of these events with GW detectors. This study is important to build a general relativistic model of eccentric binary neutron star.

The goals of this project are: (i) to develop the independent model techniques needed to robustly detect GWs from relativistic transisnt events, and determine the signal structure; (ii) to apply these to data from the Advanced LIGO / Advanced VIRGO network to detect GWs; and (iii) to use detected GWs as probes of relativistic systems and fundamental physics.

## **Resumo atividades**

During eight months of postdoc I focused my research activity mainly on my projects developed in collaboration with Riccardo Sturani. During the first two months of my postdoc I have focused the study of binary systems, in particular I derived an additional contribution, which is due to the quadrupole moments of the companions. In fact a rotating star's oblateness create a deformation in the gravitational field outside the star, which is measured by the quadrupolemomentum tensor. We derived the effect of the quadrupole moment on the orbital motion and rate of inspiral of a compact binary systems, composed of neutron stars and black holes. We find that in the case of circular orbits, the quadrupole-monopole interaction affects the relation between orbital radius and angular velocity, and also the rate of inspiral, by a quantity of order  $(v/c)^4$ , where v is the orbital velocity and c the speed of light.

In the remaining six months I have investigated the excitation of neutron stars oscillation modes by the orbital motion. We study eccentric orbits and show that tidal interaction can excite the fmode oscillations of the neutron star and compute the amount of energy and angular momentum deposited into the neutron stars by the orbital motion tidal forces. We studied the f-mode oscillations of cold neutron stars using recent microscopic nuclear equations of state (EoS), and we estimate their imprint and detectability into the emitted gravitational waves by the third generation earth-based gravitational wave interferometric detectors. We calculate the orbital phase error due to the resonant energy transfer between the binary orbit and the neutron stars oscillation mode. This work will be put on arXiv in the coming weeks and after submitted for publication to APJ.

## **Conferences and Workshops**

1. Einstein Toolkit EU-School and Workshop, 13-17 June 2016, Trento, Italy.

I have attended the Workshop and presented the seminar "Torsional oscillations of nonbare strange stars".

2. New Compstar School 2016 "Neutron Stars: Gravitational Physics, Theory & Observations", 5-9 September 2016, University of Coimbra, Portugal.

# Seminars

Seminar at ICTP-SAIFR. "Torsional oscillations of nonbare strange stars", 18/04/2016 JC Cosmology.

Seminar at Trento University. "Torsional oscillations of nonbare strange stars", 16/06/2016 .

# Scientific Report 2016

Title Postdoc Supervisor Fapesp process Period Integrabilidade em teorias de gauge Ryo Suzuki Nathan Jacob Berkovits 2015/04030-7 01/Oct/2015 - 30/Nov/2016





INTERNATIONAL CENTER FOR THEORETICAL PHYSICS SOUTH AMERICAN INSTITUTE FOR FUNDAMENTAL RESEARCH This scientific report summarizes my activity at ICTP-SAIFR during October 1st in 2015 and November 30th in 2016.

## 1 Research

Integrability is an indispensable tool to test the AdS/CFT correspondence between  $\mathcal{N} = 4$  Super Yang Mills (SYM) theory in four dimensions and superstring on AdS<sub>5</sub> × S<sup>5</sup> in the planar limit. By making full use of integrability, we can compute the energy spectrum (and other quantities) of a general class of gauge-invariant operators or string states at any values of the 't Hooft coupling  $\lambda$ .

My projects are closely related to this line of development. In large  $N_c$  gauge theories, the connected *n*-point functions typically scale as  $1/N_c^{n-2}$  as  $N_c \to \infty$ . It implies that planar higher-point functions are somehow related to the  $1/N_c$  corrections to the spectrum. However, it is not known how to naturally generalize the planar integrability of  $\mathcal{N} = 4$  SYM at finite  $N_c$ . What we need is to develop mathematical tools for the study of non-planar structure in the loop-level spectrum and tree-level correlation functions.

#### **1.1** Correlation functions at finite $N_c$

General gauge-invariant on-shell local operators of  $\mathcal{N} = 4$  SYM can be written as

$$\mathcal{O}_{\gamma}^{A_1\dots A_L} = (W^{A_1})_{a_{\gamma(1)}}^{a_1} (W^{A_2})_{a_{\gamma(2)}}^{a_2} \dots (W^{A_L})_{a_{\gamma(L)}}^{a_L} \equiv \operatorname{tr}_L(\gamma W^{\bar{A}}), W^A = \{ D^S F, D^S \psi, D^S \phi, D^S \bar{\psi}, D^S \bar{F} \},$$
(1)

where  $\gamma$  is an element of the permutation group  $S_L$  and  $W^A$  is called  $\mathcal{N} = 4$  alphabet.  $\mathcal{O}_{\gamma}^{\vec{A}}$  is a single-trace operator if the permutation  $\gamma$  has the cycle structure (12...L). The equation (1) specifies a unique operator for each  $\gamma$  and  $\vec{A}$  modulo the equivalence relation

$$\mathcal{O}_{\gamma}^{A_1\dots A_L} = \mathcal{O}_{\sigma\gamma\sigma^{-1}}^{A_{\sigma(1)}\dots A_{\sigma(L)}}, \qquad (\sigma \in S_L).$$
<sup>(2)</sup>

This description of multi-trace operators is called *permutation basis* in the literature.

Traditionally in AdS/CFT we associate a single closed string state to a single-trace operator of a large  $N_c$  gauge theory, or a single periodic spin-chain state of an integrable model. In the permutation basis, any multi-trace operator is collectively described by a single permutation  $\gamma$ , as shown in Figure 1.



Figure 1: Spin chain state in the permutation basis.

What is the similarity and difference of two descriptions? For a clear answer, we should study the correlation functions of operators in a specific sector in detail.

In [1] we considered  $SO(N_f)$  mesonic singlets. The mesonic singlets form a closed sector under the one-loop operator mixing, and are given by

$$\mathcal{O}_{\alpha} = \operatorname{tr}_{2n} \left( \alpha \ \Phi_{a_1} \otimes \Phi_{a_1} \otimes \Phi_{a_2} \otimes \Phi_{a_2} \otimes \cdots \otimes \Phi_{a_n} \otimes \Phi_{a_n} \right), \qquad (a_k = 1, 2, \dots, N_f)$$
(3)

This operator is invariant under the action of the wreath-product group  $\sigma \in S_n[S_2]$  in the sense of (2). The  $\mathcal{N} = 4$  SYM corresponds to the case of  $N_f = 6$ , but it is convenient to work at general  $N_f$ . The tree-level two-point functions in the permutation basis are given by

$$\langle \mathcal{O}_{\alpha_1} \mathcal{O}_{\alpha_2} \rangle = \sum_{\beta_1 \in S_{2n}} \sum_{\beta_2 \in S_{2n}} \sum_{\sigma \in S_{2n}} N_c^{C(\beta_1)} N_f^{\frac{1}{2}C(\beta_2)} \delta_{2n} (\beta_1^{-1} \alpha_1 \sigma \alpha_2 \sigma^{-1}) \delta_{2n} (\beta_2^{-1} \sigma \Sigma_0 \sigma^{-1} \Sigma_0).$$
(4)

where  $C(\sigma)$  counts the number of cycles in  $\sigma$ ,  $\delta_{2n}(\sigma) = 1$  if  $\sigma = 1$  and vanishes otherwise, and  $\Sigma_0$  is a fixed permutation  $\Sigma_0 = (1, 2)(3, 4) \dots (2n - 1, 2n)$ . The trace of (4) over the Hilbert space counts the number of gauge-invariant operators, at large  $N_c$  and large  $N_f$ .

We can interpret (4) geometrically as follows. Consider a topological lattice gauge theory with the finite gauge group  $S_{2n}$ . The gauge fields live on the edges of the lattice, taking values on  $S_{2n}$ . The observables of this theory are associated to each 2-cell of the lattice, whose expectation value is given by  $\delta_{2n}(e_1e_2...)$ , where  $e_i$  are the edge degrees of freedom surrounding the 2-cell. A collection of 2-cells makes a (singular) 2-manifold  $M_2$  shown in Figure 2. Roughly speaking,  $M_2$  represents the structure of Wick contractions behind the tree-level two-point functions (4). The precise relation between the geometry of  $M_2$  and string worldsheet is under investigation.



Figure 2: Tree-level two-point functions as an observable of a topological lattice gauge theory whose target manifold is  $M_2$  with boundaries  $(\alpha_1, \alpha_2)$  and defects  $(\Sigma_0, \beta_1, \beta_2)$ .

Whenever the operator length exceeds  $N_c$ , we need to solve finite  $N_c$  constraints to obtain a linearly independent set of operators. By the finite N constraints we mean the following identity:

$$0 = \sum_{\sigma \in S_L} \operatorname{sign}(\sigma) X_{i_{\sigma(1)}}^{(1)} X_{i_{\sigma(2)}}^{(2)} \dots X_{i_{\sigma(L)}}^{(L)}, \qquad (i_k = 1, 2, \dots, N < L).$$
(5)

Namely, if you anti-symmetrize L indices of a tensor whose index runs from 1 to N < L, then this tensor vanishes. Similarly we have finite  $N_f$  constraints, which become important if the operator length is greater than  $2N_f$ .

It is quite non-trivial to solve the constraints (5) in the permutation basis. A well-known trick is to rewrite the permutation basis into representation basis by using Fourier transform on finite groups,

$$\mathcal{O}^{R,\Lambda_1,\tau} = \sum_{\alpha \in S_{2n}} B_k^{\Lambda_1} S^{\tau,\Lambda_1 RR}_{\ k \ i \ j} D^R_{ij}(\alpha^{-1}) \mathcal{O}_{\alpha} , \qquad (6)$$

$$\langle \mathcal{O}^{R,\Lambda_1,\tau} O^{S,\Lambda_1',\tau'} \rangle = \delta^{RS} \,\delta^{\Lambda_1\Lambda_1'} \,\delta^{\tau\tau'} \,\left(\frac{(2n)!}{\dim_{S_{2n}}(R)}\right)^2 \dim_{U(N_c)}(R) \,\omega_{\Lambda_1/2}(N_f),\tag{7}$$

where R,  $\Lambda_1$  are irreducible representations of  $S_{2n}$ ,  $\tau$  is a multiplicity label in the irreducible decomposition  $R \otimes R = \bigoplus_{\Lambda_1} \Lambda_1^{\otimes \tau}$ .  $D_{ij}^R(\alpha^{-1})$  is the representation matrix of  $\alpha \in S_{2n}$ , and the  $S^{\tau, \Lambda_1 RR}_{k i j}$  is the Clebsch-Gordan coefficient of  $S_{2n}$ . The branching coefficient  $B_k^{\Lambda_1}$  is defined via the reduction of the irreducible representation  $\Lambda_1$  of  $S_{2n}$  in terms of a direct sum of irreducible representations of  $S_n[S_2] \subset S_{2n}$ . The dim<sub>G</sub>(R) is the dimension of R as the representation of group G, and  $\omega_{\Lambda_1/2}(N_f)$ is the zonal spherical function for the Gelfand pair  $(GL(N_f), O(N_f))$  in the representation  $\Lambda_1/2$ .<sup>1</sup>

The operators in the representation basis (6) have several remarkable properties:

- It diagonalizes the tree-level two-point functions at finite  $N_c$ . This is true even if we twist  $U(N_c)$  or  $SO(N_f)$  Wick contraction rules, because all coefficients are written purely in terms of the quantities of finite group theory.
- Our representation basis coincides with the specialization of another orthonormal basis called covariant basis.<sup>2</sup>
- The finite  $N_c$  or finite  $N_f$  constraints are easily solved by the conditions

$$c_1(R) \le N_c \qquad c_1(\Lambda_1) \le N_f \,, \tag{8}$$

where  $c_1(R)$  is the number of rows in the Young diagram R.

At one-loop, neither the permutation nor representation basis diagonalizes the dilatation operator at finite  $N_c$ . The equation (2) says that all planar operator mixing is an adjoint action of  $S_L$ ,  $\gamma \mapsto \sigma \gamma \sigma^{-1}$ . Non-planar mixing involves complicated "non-linear" transformations of  $S_L$ .<sup>3</sup> This nonlinearity explains why the standard basis of  $\mathbb{C}[S_L]$  is not useful for diagonalizing non-planar dilatation.

<sup>&</sup>lt;sup>1</sup>I. G. Macdonald, "Symmetric functions and Hall polynomials," Oxford Univ. Press, Oxford, 2nd Edition (1995). <sup>2</sup>T. W. Brown, P. J. Heslop and S. Ramgoolam, "Diagonal Free Field Matrix Correlators, Global Symmetries and

Giant Gravitons," JHEP 0904 (2009) 089, doi:10.1088/1126-6708/2009/04/089 [arXiv:0806.1911 [hep-th]].

<sup>&</sup>lt;sup>3</sup>S. Bellucci, P. Y. Casteill, J. F. Morales and C. Sochichiu, "Spin Bit Models from Nonplanar  $\mathcal{N} = 4$  SYM," Nucl. Phys. B **699** (2004) 151, doi:10.1016/j.nuclphysb.2004.07.025 [hep-th/0404066].

#### **1.2** Four-point functions

There is a resurge of interest in conformal bootstrap techniques, which allows us to compute fourpoint functions of general conformal field theories. The goal of this project is to understand the precise relation between the connected four-point functions and the  $1/N_c$  corrections to the spectrum of perturbative  $\mathcal{N} = 4$  SYM. We expect that the integrability methods will eventually allow us to construct planar four-point functions. Yet it is unclear how to extract efficiently the information about the spectrum.

By taking the OPE limit of 4-point functions of scalar BPS operators, we obtain a set of average anomalous dimensions of the intermediate operators propagating the internal line. The averaging weight is given by the OPE coefficients squared. When the three-point coupling is extremal, we obtain non-planar corrections to the multi-trace operators as shown in Figure 3.



Figure 3: Decomposing four-point functions into a two-point function and two three-point functions.

If the intermediate operators are made out of scalars only, we find that the average anomalous dimensions do not match the OPE limit of the perturbative four-point function. This finding would imply that there are missing superconformal primaries containing covariant derivatives. There should be multiple superconformal primaries of this type, which undergo operator mixing. However, it is quite tedious to enumerate all possible superconformal primaries and solve the operator mixing problem, due to the intricate structure of spinor indices. I am investigating how to overcome such technical difficulty.

#### **1.3** Lecture note on superstring

This is not an initially planned project, but came up in with the motivation for learning better the amplitudes of  $AdS_5 \times S^5$  superstring. In 2016, Prof. Berkovits gave a series of lectures about superstring theories at ICTP-SAIFR. The lectures reviewed Ramond-Neveu-Schwarz, Green-Schwarz and Pure-Spinor formalisms, and explained a recent reformulation of Pure-Spinor.<sup>4</sup> Together with graduate students, I am summarizing and typesetting the lecture note.

<sup>&</sup>lt;sup>4</sup>N. Berkovits, "Untwisting the Pure Spinor Formalism to the RNS and Twistor String in a Flat and  $AdS_5 \times S^5$  Background," JHEP **1606** (2016) 127, doi:10.1007/JHEP06(2016)127 [arXiv:1604.04617 [hep-th]].

## 2 Publication

[1] Y. Kimura, S. Ramgoolam and R. Suzuki, "Flavour singlets in gauge theory as Permutations," arXiv:1608.03188 [hep-th] (to appear in JHEP).

## 3 Seminars, workshops and conferences

Below is the list of workshops and conferences I participated in 2016:

- gave a short talk at School on Fundamental Aspects of String Theory in ICTP-SAIFR, May 23 30. http://www.ictp-saifr.org/?page\_id=10349
- attended VIII Workshop on String Field Theory and Related Aspects in ICTP-SAIFR, May 31 June 3. http://www.ictp-saifr.org/?page\_id=10351
- attended Workshop on Mathematical Physics in ICTP-SAIFR, June 16 17. http://www.ictp-saifr.org/?page\_id=11263
- gave a talk at *YITP workshop*, *Strings and Fields* in Yukawa Institute for Theoretical Physics, Aug 8 - 12. http://www2.yukawa.kyoto-u.ac.jp/ qft.web/
- gave a talk at *KEK Theory Seminar* in KEK High Energy Accelerator Research Organization, Aug 18. http://www2.kek.jp/theory-center/theory/seminars/
- gave a poster presentation at *Integrability in Gauge and String Theory 2016* in Humboldt Universität zu Berlin, Aug 22 26. http://igst2016.physik.hu-berlin.de
- organized a session and gave a talk at Workshop on 3-point functions in Gauge/String theories in ICTP-SAIFR, Sep 19 30. http://www.ictp-saifr.org/?page\_id=12169

## 4 Organization of journal clubs

I organized journal club in Quantum Field Theory and String Theory. This journal club started in 2015, and we continued the meeting in 2016. In 2015 we had four talks, and in 2016 we had six. The talks are intended for introducing recent papers to graduate students and postdocs. The topics include holography, blackholes, AdS/CFT, integrability, chaos and twistors.

## 5 Reviewer for international journals

I undertook the reviewing of articles in the following journals:

- Nuclear Physics B
- JHEP

# **FAPESP SCIENTIFIC REPORT** 2016

# Phenomenology of the Large Hadron Collider

Postdoc: Alberto Tonero Supervisor: Nathan J. Berkovits FAPESP Process: 2013/02404-1 Period: 01/04/2015 to 30/11/2016

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**ICTP-SAIFR & IFT-UNESP** São Paulo

# Resumo do projeto

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.

# **Resumo atividades ano 2013**

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 guark 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

- M. Fabbirichesi, M. Pinamonti and A. Tonero, "*Stringent limits on top-quark compositeness from tt production at the LHC*", arXiv:1307.5750 [hep-ph], *Phys.Rev. D89 (2014) 7, 074028*.

## Conferences and workshops

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

- "5<sup>th</sup> 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.

# **Resumo atividades ano 2014**

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

- R. Rosenfeld and A. Tonero, "*Dipole-induced anomalous top quark couplings at the LHC*", arXiv:1404.2581 [hep-ph], *Phys.Rev. D90 (2014) 1, 017701*.

- M. Fabbrichesi, M. Pinamonti and A. Tonero, "*Limits on anomalous top quark gauge couplings from Tevatron and LHC data*", arXiv:1406.5393 [hep-ph], *Eur.Phys.J. C74 (2014) 12, 3193*.

## Conferences and workshops

- "Origin of Mass 2014", 19-22 May 2014, Odense, Denmark.
- "Planck 2014", 26-30 May 2014, Paris, France.
- "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, Medellin, Colombia.

# **Resumo atividades ano 2015**

During the year 2015 my research activity was focused mainly on projects related to LHC phenomenology and formal aspects of 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  $Z_2$  –scalar theories. This work has been presented in the E-print arXiv:1504.00225 and has been published in *Phys.Rev. D94* (2016) 2, 025015.

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 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. This work has been presented in the E-print arXiv:1505.03119 and has been published *Eur. Phys. Journ. C76 (2016) 4, 226*.

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. 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  $pp \rightarrow l vl l vl jj$ . 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<sup>-1</sup> 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 W W  $\rightarrow$  W W 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 published in *Phys.Rev. D93 (2016)* 1, 015004.

## Preprints and publications

- A. Codello and A. Tonero, "*Renormalization group improved computation of correlation functions in theories with nontrivial phase diagram*", arXiv:1504.00225 [hep-th], *Phys.Rev. D94 (2016) 2, 025015*.

- A. Codello, R. Percacci, L. Rachwal and A. Tonero, "*Computing the effective action with the functional renormalization group*", arXiv:1505.03119 [hep-th], *Eur.Phys.J. C76 (2016) 4, 226*.

- 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], *Phys. Rev. D93* (2016) 1, 015004.

## Conferences and workshops

- Workshop "Physics at TeV colliders", 10-19 June 2015, Les Houches, France.

- "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) on the project related to the optimization of shape analysis for SM higher dimensional operators at the LHC.

# Atividades de pesquisa ano 2016

During the year 2016 I focused my research activity mainly on two projects.

The first project I have completed in 2016 was realized in collaboration with R. Rosenfeld (IFT-UNESP), Christoph Englert (Glasgow University) and Michael Spannowsky (Durham University) and was related to 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 have investigated 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+l-, 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. In this paper we have re-investigate electroweak signal-background interference in associated Higgs production via gluon fusion in the presence of new physics in the top Higgs sector. Considering the full final state pp  $\rightarrow$ bbl+l- (  $l=e, \mu$ ), we discuss how new physics in the top Higgs sector that enhances the ZZ component can leave footprints in the HZ limit setting. In passing we investigate the phenomenology of a class of new physics interactions that can be genuinely studied in this process. 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 work has been presented in the E-print arXiv:1603.05304 and has been published in *Europhys.Lett.* 114 (2016) 3, 31001.

The second project I have completed in 2016 was realized in collaboration with S. Fichet (IFT-UNESP) and P. R. Teles (CMS and CBPF). When the Standard Model is interpreted as the renormalizable sector of a low-energy effective theory, the effects of new physics are encoded into a set of higher dimensional operators. These operators potentially deform the shapes of Standard Model differential distributions of final states observable at colliders. We describe a simple and systematic method to obtain optimal estimations of these deformations when using numerical tools, like Monte Carlo simulations. A crucial aspect of this method is minimization of the estimation uncertainty: we demonstrate how the operator coefficients have to be set in the simulations in order to get optimal results. The uncertainty on the interference term turns out to be the most difficult to control and grows very quickly when the interference is suppressed. We exemplify our method by computing the deformations induced by the O<sub>3W</sub> operator in W + W – production at the LHC, and by deriving a bound on O<sub>3W</sub> using 8 TeV CMS data. This work has been presented in the E-print arXiv:1611.01165 and has been submitted for publication to *JHEP*.

# Preprints and publications

- C. Englert, R. Rosenfeld, M. Spannowsky and A. Tonero, "*New physics and signal-background interference in associated pp*  $\rightarrow$  *HZ production*", arXiv: 1603.05304 [hep-ph], published in *Europhys.Lett.* **114 (2016) 3, 31001.** 

- S. Fichet, P. R. Teles and A. Tonero, "On the optimal determination of differential rates in the presence of higher-dimensional operators", arXiv:1611.01165 [hep-ph].

## Conferences and workshops

- "Planck 2016", 23-27 May 2016, Valencia, Spain.

- "Encontro de Física 2016", 03-07 September 2016, Natal, RN, Brazil.

- "Program on particle physics at the New Energy Frontier of 13 TeV", from October 3 to November 11, ICTP-SAIFR, São Paulo, SP, Brazil.

## Special seminars

- Seminar at UFPB *"Constraints on new physics at the LHC using effective field theory"*, 9 September 2016, João Pessoa, Paraiba, Brazil.

- Seminar at UFABC *"Constraints on new physics at the LHC using effective field theory"*, 28 September 2016, Santo André, SP.

## Visiting

I spent two weeks visiting the CERN Theory Group in June 2016 under the agreement between the ICTP-SAIFR and CERN Theory Group. During that period I took the opportunity to start working with A. Urbano (CERN theoretical division) on topics related to new physics signatures at the LHC run II.