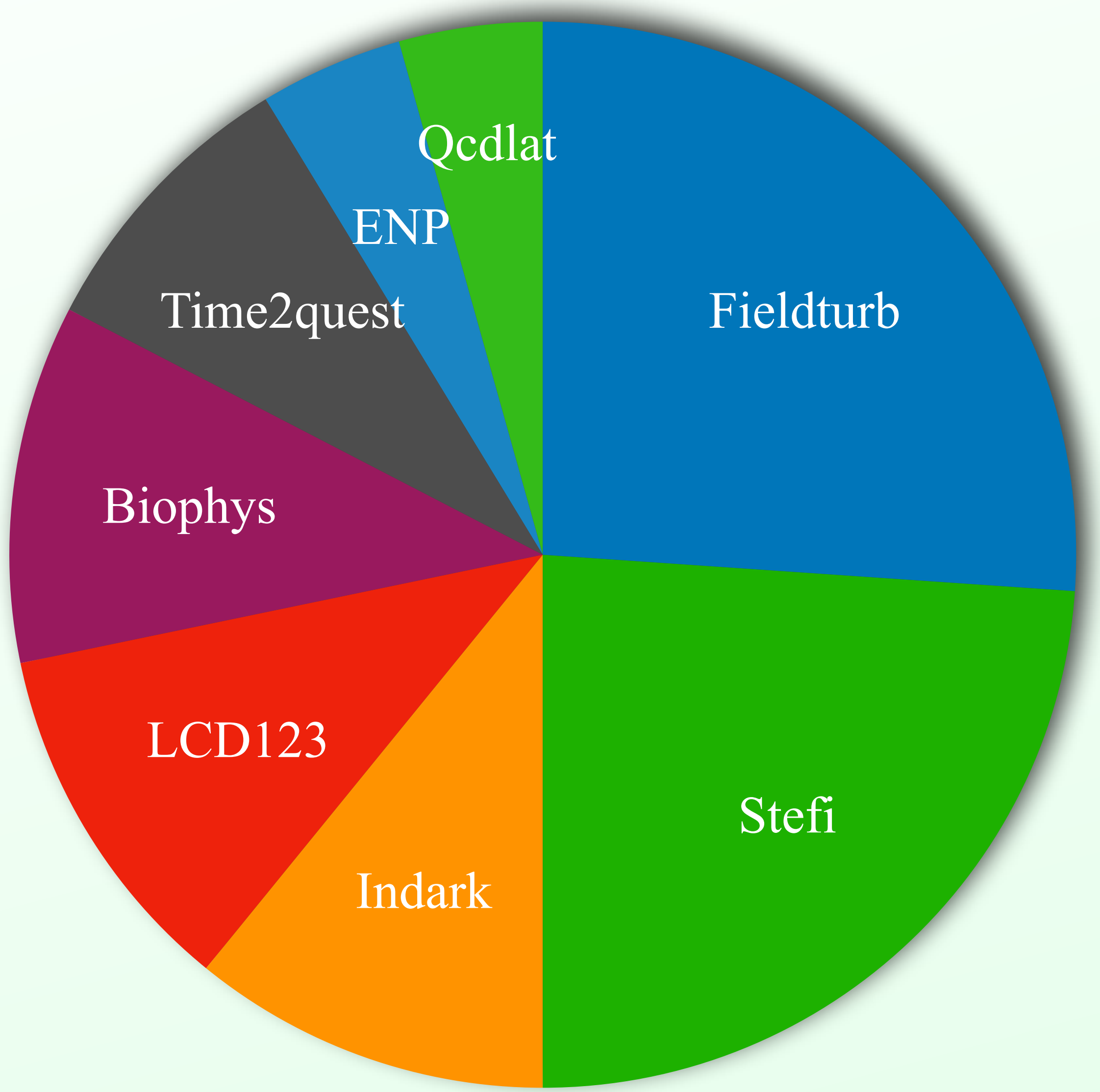
INFN Istituto Nazionale di Fisica Nucleare
SEZIONE DI ROMA TOR VERGATA

Preventivi 2022
Gruppo IV

Iniziative Specifiche

- FTE:



- FIELDTURB: Sistemi complessi, turbolenza
  Massimo Cencini, ricercatori: 15, FTE 14
- STEFI: Teoria di stringa, gauge e gravita
  Gianfranco Pradisi ricercatori: 12, FTE 10.3
- LQCD123: Teorie di gauge sul reticolo
  Nazario Tantalo ricercatori: 7, FTE 5.5
- BIOPHYS: Biofisica
  Silvia Morante ricercatori: 7, FTE 5.5
- INDARK: Cosmologia
  Marina Migliaccio ricercatori: 11, FTE 6.1
- Time2quest: Struttura della materia
  Gianluca Stefanucci ricercatori: 6, FTE 6
- ENP: Fisica standard model e beyond
  Giulia Maria de Divitiis ricercatori: 3, FTE 1.75
- QCDLAT: QCD sul reticolo
  Tassos Vladikas ricercatori: 4, FTE 3

FieldTurb

Responsabile locale: Massimo Cencini
Nazionale: Guido Boffetta (To)

1 Agasthya Lokahith PHD 100
2 Benzi Roberto PO 100
3 Biferale Luca PO 70
4 Bonaccorso Fabio PHD 70
5 Buzzicotti Michele RTDA 100
6 Cencini Massimo CNR 50
7 Cimini Giulio RTDB 100
8 De Toma Vincenzo PHD 100
9 Goedert Guilherme PHD 100
10 Guglietta FabioPHD 100
11 Marra Rossana PO 100
12 Capocci Damiano PHD 100
13 Puglisi Andrea Primo Ricercatore 50
14 Sbragaglia Mauro PA 100
15 Heinnen Robin postdoc 100

Numero Totale Ricercatori 15 FTE: 14

Attivita':
In the context of complex fluids, we have: completed a set of studies on immiscible Rayleigh-Taylor systems by using Lattice Boltzman Methods; demonstrate that the multi-phase lattice Boltzmann method (LBM) yields a curvature dependent surface tension σ by means of three-dimensional hydrostatic droplets/bubbles simulations; studied loading and relaxation dynamics of a red blood cell ; rationalized the power law scaling of stress and strain overshoots in soft glassy material.
We have demonstrated the potentialities of entropic LBM for Direct Numerical Simulations of 3D turbulent flows.

We have also investigated by using a coarse graning techniques geophysical fluids showing its usefulness in decomposing surface geostrophic kinetic energy in the global ocean.
In the context of active matter, we have demonstrated that models with Viksec-like interactions are close to optimality with respect to the goal of collision avoidance, and investigated the fluctuation dissipation relation.

We have further developed our research in AI and Machine Learning. In particular, we have shown how to reconstruct incomplete information on complex velocity fields using deep generative models, and shown how active swimmers can learn non trivial pursuing-evasion strategies by using Reinforcement Learning and hydrodynamical cues.

In the context of Machine Learning applications we plan to continue the research line on the use of Reinforcement Learning to the navigation and accomplishment of other tasks by active swimmers in complex flows. To apply Reservoir Computing and Deep Learning for testing their potentialities in the reconstructing Lagrangian statistics and for exploring intermittency in shell models of turbulence.

We will continue the analytical and numerical investigation of active tubulence in complex fluids. We will study in particular the effect of inertial particles on the instabilitues of a channel flow and of active particles on the large scale properties of the flow. Moreover, we shall continune our exploration on the interplay between fluid transport and self-propulsion in different flow and swimming configurations.

We shall continue our research of complex fluids, emulsions and droplets exploring their glassy behavior with multiphase LBM.

Richiesta: 21KE

Resp. Locale: G Pradisi
Resp. Naz: G. Bonelli

STEFI

Anagrafica:

1. Massimo Bianchi, PO, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)
2 Dario Consoli, assegnista, Universita' di Roma "Tor Vergata" (100%)
3. Giuseppe D'Appollonio, RTI, Dip. Fisica , Universita' di Cagliari (80%)
4. Giorgo di Russo, PhD, Universita' di Roma "Tor Vergata" (100%)
5. Francesco Fucito, DdR INFN, Sezione di Roma "Tor Vergata" (100%)
6. Francisco Morales, PR INFN, Sezione di Roma "Tor Vergata" (100%)
7. Gianfranco Pradisi, PA, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)
8. Fabio Riccioni, Dip. Fisica, Universita' di Roma "Sapienza" (100%)
9. Salvo Mancani, Dip. Fisica, Universita' di Roma "Sapienza" (100%)
10. Alberto Salvio, RTD B, Dip. Fisica, Universita' di Roma "Tor Vergata" (25%)
11. Raffaele Savelli, PA, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)
12. Alfredo Grillo, PhD student, Dip. Fisica, Universita' di Roma "Tor Vergata" (100%)

Numero ricercatori: 12, FTE: 10.3

- D-brane probes of (un)oriented CY singularities and identification of new IR fixed points.
- Fuzz-ball phenomenology by exploring their multi-polar structure, light-rings, Lyapunov exponents, Quasi Normal Modes and GW echoes
- String corrections to gravitational and electro-magnetic memories, including spin effects.
- Systematics of alpha' corrections to 4d effective actions coming from F-theory compactifications.
- New four-dimensional conformal field theories arising from probing S-fold geometries in String Theory.
- Computation of higher-derivative corrections to Type IIB supergravity, from loops in 11 dimensions.
- Computation of Donaldson invariants of toric manifolds.
- Study of D(-1)-D7 brane system in presence of background fields.
- Computation of the OPE coefficients for supersymmetric theories with conformal invariance, conformal bootstrap.
- Gravitational scattering of ultra-relativistic elementary particles and strings, from numerical and analytical GR to QFT.
- Beyond the standard model scenarios that are valid over a vast energy range: from the Hubble up to the Planck scale.
- Study of the reheating phase in inflationary models with an inflaton fluid exhibiting variable EoS.

Richiesta: 20 KE

LQCD123

Phenomenology with Lattice QCD in Roma123

Responsabile nazionale: Vittorio Lubicz (Roma Tre)
Responsabile locale: Nazario Tantalo

Anagrafica

1) Roberto Frezzotti (PO 50%)
2) Marco Guagnelli (R INFN 100%)
3) Giancarlo Rossi (PO 0%),
4) Nazario Tantalo (PA 100%)
5) Madeleine Dale (PhD, D)
6) Floriano Manigrasso(PhD, D)
7) Antonino Todaro(PhD, D)

Ricercatori: 7, FTE: 5.5

Attività' scientifica

The activity of our group is focused on challenging non-perturbative lattice computations. These include leading isospin breaking and QED radiative corrections to hadronic observables, needed to perform precision tests of the Standard Model, as well as non-perturbative investigations of new physics models with new strong interactions. In particular, we have

- computed the ratio of kaon and pion leptonic decay constants in N_f=2+1+1 QCD;
- performed out a state-of-the-art calculation of the up, down, strange and charm quark masses within the lattice (isosymmetric) QCD framework;
- proposed a scheme of lattice twisted-mass fermion regularization which is particularly convenient for application to isospin breaking (IB) QCD and QED calculations;
- computed the electric dipole moment of the neutron from first-principles by performing Nf=2+1+1 lattice simulations;
- determined the $\Delta(1232)$ resonance parameters using lattice QCD and the Lüscher method;
- presented a new method, based on Gaussian process regression, for reconstructing the continuous x-dependence of parton distribution functions (PDFs) from quasi-PDFs computed using lattice QCD;
- performed a calculation of isovector unpolarized and helicity PDFs using lattice ensembles with N_f=2+1+1 Wilson twisted mass fermions;
- evaluated for the first time on the lattice the radiative leptonic decays of a pseudoscalar meson P-> l nu gamma, where P is a pion, kaon, D or D_s meson and gamma is a real photon. We have also presented a detailed phenomenological analysis in which our first-principles non-perturbative results for the decay rates pi-> l nu gamma and K-> l nu gamma have been compared with the existing experimental data;
- established from first principles the existence of a non-perturbative mechanism leading to elementary particle mass generation in models with gauge fields, fermions and scalars if an exact invariance forbids power divergent fermion masses and fermionic chiral symmetries broken at UV scale are maximally restored;

RESEARCH PROGRAM 2022

- QED and isospin breaking corrections to the neutron beta decay, which, once combined with the measured value of the neutron's lifetime, allows a precise determination of Vud. We will also compute the rate for the semileptonic charged pion decay including QED radiative corrections;
- Extend the computation of the form factors for the radiative leptonic decays of pseudoscalar mesons to the case of B mesons and to the case of rare decays mediated by a virtual photon;
- Generate configurations of non-perturbative QCD+QED with C-parity boundary conditions.
- Hadronic spectral densities from euclidean correlators, evaluate the inclusive decay rate B->Xc l nu and extract the CKM matrix element Vcb;
- Dynamical generation of the electroweak scale, universality of the physical observables in a recently proposed non-perturbative mechanism for the origin of the masses of the elementary particles from new superstrong interactions (possibly leading to a composite Higgs scenario).

RICHIESTA: 10 KE

Biophys

Title: Intrinsically disordered proteins: multi-level computational approaches

Responsabile Nazionale: Mario Nicodemi
Responsabile Locale: Silvia Morante
Anagrafica:

1) Simone Botticelli, assegnista, 100%
2) La Penna Giovanni, PR, 50%
3) Minicozzi Velia, R 100%
4) Morante Silvia, PO, 100%
5) Nobili Germano, PhD, 100%
6) Rossi Giancarlo, PO
7)Stellato Francesco, R, 100%

Ricercatori 7 FTE 5.5 (totale)

Attività' scientifiche:

Intrinsically disordered proteins: multi-level computational approaches
Computational methods are widely employed to determine the structure and the dynamics of biologically relevant molecules such as proteins. We are applying these methods to study the intrinsically disordered proteins (IDPs), which are flexible, active proteins that can be associated with human diseases such as cancer, cardiovascular pathologies, neurodegenerative diseases and diabetes. Conformational flexibility and structural plasticity may be a benefit, allowing IDPs to switch from a biological role to another. Molecular Dynamics (MD) is a multi-scale approach that goes from coarse-grained MD to all atoms classical and *ab initio* calculations. Proteins are made of a large number of atoms and *ab initio* quantum-mechanical approaches are often compulsory (e.g. when the knowledge of the role played by metal ions is an essential ingredient). This is why HPC platforms and innovative theoretical and computational methodologies are required. MD is also exploited to analyze experimental results coming from Large Scale facilities such as synchrotrons and Free Electron Lasers.
Our field of investigation are:
a) Protein aggregation
We exploit computational (classical and *ab initio* MD) and experimental (X-ray absorption spectroscopy - XAS) techniques to shed light on the IDP aggregation phenomenon, in particular on the influence that metal ions and small molecules can have in the progression of neurodegenerative diseases.
b) The role of mutations in protein stability
We integrate computational approaches with experiments to assess the impact of a number of given mutations on proteins known to be associated to cancer and genetic diseases. Our study is aimed at measuring the impact of single mutations in Frataxin, a protein associated to the Friedrich ataxia (a rare but well investigated neurodegenerative disease) by estimating stability differences between mutated and native (wild-type) proteins. The impact of single mutations on protein stability can be assessed from non-equilibrium MD simulations performed with the multiple-walkers metadynamics method. This work is part of the PRIN n. 201744NR8S:"Integrative tools for defining the molecular basis of the diseases: computational and experimental methods for protein variant interpretation".
c) The interaction of metal ions with SARS-COVID-19 proteins
In order to unravel the role of metal ions in the SARS-COVID-19 infection, we employ classical MD to model the interaction between Zn(II) cations, two accessory SARS-COVID-19 proteins (ORF7a and ORF8) and BST2-tetherin antigen [Morante *et al.* Front. Mol. Biosci. 2020]. The best supported hypothesis proposed for the orf7a and orf8 protein function is based on their ability to interfere with virion budding operated by the cellular BST2-tetherin antigen. We are performing MD simulations of the orf7a/BST2 and orf8/BST2 complexes in the presence and in the absence of Zn(II) to determine if and how Zn can affect the stability of such systems thus possibly impeding the correct immune response.
e) The stability of trimeric proteins.
We use a combined theoretical and computational approach aimed at understanding the stability of trimeric proteins in which the direct calculation of structural and topological properties of the system is complemented and compared to results coming from all-atom simulations. Fluorescence spectroscopy experiments are in line with our numerical results.

Richiesta in KE: 8 KE

INDARK

Title: Inflation, Dark Matter and the Large-Scale Structure of the Universe

Responsabile Nazionale: Massimiliano Lattanzi (INFN Ferrara)
Responsabile Locale: Marina Migliaccio
Anagrafica:

1) Hervé Bourdin (RTD-B UniRM2) 50%
2) Giancarlo De Gasperis (Ric. Univ UniRM2) 20%
3) Pasquale Mazzotta (PO UniRM2) 50%
4) Marina Migliaccio (Coord., RTD-B UniRM2) 50%
5) Nicola Vittorio (PO UniRM2) 50%
6) New RTD-A UniRM2 80%
7) Alessandro Carones (Ph.D. student UniRM2) 30%
8) Federico De Luca (Ph.D. student UniRM2) 80%
9) Filippo Oppizzi (Post-doc UniRM2) 80%
10) Giacomo Galoni (PHD) 60%
11) Giulia Piccirilli (PHD) 60%

Ricercatori 11, FTE 6.1

Attività' scientifiche:

The focus of the research project is to investigate crucial aspects of the standard cosmological model and its extensions, and their connection with particle physics.

The main research topics are organized as follows:

i. Inflation and the primordial universe.
ii. Dark Matter, Neutrinos and other Light Relics.
iii. Dark Energy and Modified Gravity.
iv. Cosmological observables as a probe of fundamental physics.

We plan to interpret the combined information from present and future observations of Cosmic Microwave Background (CMB) radiation, Large-Scale Structure (LSS) of the Universe, gravitational wave (GW) signals, and other cosmological probes in light of these models, and to sharpen the theoretical tools that allow such an interpretation. To this purpose, a wide range of techniques are employed, including theoretical modelling of the cosmological evolution (using both analytical and numerical methods), analysis and interpretation of available data, together with simulation of mock data samples for future experiments. Merging the complementary expertise present in the different research units (RU) involved in the project allows to design a comprehensive, multiprobe-multiscale, approach.

In this framework, the Roma2 RU will: i) Devise novel tests of the cosmological model exploring the synergy of CMB and LSS cosmological datasets, including their cross-correlations. In preparation for future CMB missions (such as LiteBIRD, SO, CMB-S4) and galaxy surveys (like Euclid), we will assess the capability of measurements of the cross-correlation between CMB anisotropies and galaxy clustering to constrain Dark Energy and Modified Gravity models. We will also develop estimators for measuring the correlation of CMB lensing with galaxy counts, cosmic shear and cosmic filaments reconstructions in order to map the distribution of Dark Matter in the Universe and constrain models for the growth of structures. ii) Forecast the capability to constrain models of inflation with future CMB polarization data and GW measurements. iii) Search for viable solutions to the recently found tensions between measurements of the Hubble constant from early- and late-time Universe observations. These tensions are still unexplained and could hint to new physics beyond the standard model of cosmology. In particular, we will be in charge to develop new approaches to measure the Universe expansion rate with galaxy clusters.

Richiesta in KE: 13 KE

TIME2QUEST

Title: Advanced Theoretical methods for emerging 2D materials in Quantum Information Technology Studies

Responsabile Nazionale: Stefano Bellucci
Responsabile Locale: Gianluca STEFANUCCI

Anagrafica:
1) Gianluca Stefanucci (PA) - 100%
2) Enrico Perfetto (RTDB) - 100%
3) Olivia Pulci (PA) - 100%
4) Maurizia Palummo (PA) - 100%
5) Sara Postorino (PhD) - 100%
6) Simone Brozzesi (PhD) -100%

Ricercatori 6, FTE 6.0

Attività' scientifiche:
A first line of research has been devoted to the characterization, through ab-initio theoretical computational methods of ground and excited states, of the excitonic properties of several two-dimensional and layered materials of interest for electronic, opto-electronic and quantum-computation applications. In particular
1. The electronic, optical properties and radiative recombination times of gC3N4 have been calculated by means of GW and Bethe-Salpeter equation.
2. The absorption spectrum, stationary and time resolved, of a two-dimensional hybrid persovskite PEA2SnI4 is due to excitons belonging to two different series produced by a distortion of th inorganic layers due to the interaction with the organic components of the material and not, as could be supposed, by the different type of spin-orbit interaction produced by the presence of S instead of Pb, usually used.
3. The effect of the spin-orbit interaction, usually treated in a perturbative way, has been introduced in a non-collinear formulation not only at the DFT level but also at the GW and BSE level. comparison with the perturbative approach has been made for the case of TMDs monolayers.
4. The absorption and emission of pristine-like semiconducting monolayers of BN, AlN, GaN, and InN. We find exciton radiative lifetimes ranging from tenths of picoseconds (BN) to tenths of nanoseconds (InN) at room temperature, thus making 2D nitrides, especially InN, promising materials for light-emitting diodes and high-performance solar cells.
5. Topological Weyl semimetals have been studied by means of ab initio band structure methods and model Hamiltonians. The electronic, spin and topological properties of four monopnictides crystallizing in body-centered tetragonal structure have been determined. We have shown that the Weyl bands around a Weyl point W1 or W2 possess a strong anisotropy and tilt of the accompanying Dirac cones. We have found a special strain configuration on graphene that generates only the electric field, while the pseudomagnetic field is absent. Then, applying a real magnetic field, one should be able to realize experimentally the spectacular phenomenon of the collapse of Landau levels in graphene or related two-dimensional materials.

A second line of reaseach has been devoted to the nonequilibrium exciton superfluids. We have investigated their stability agains phonon-induced decoherence and screening, highlighting th signatures of this exotic phase of matter in time-resolved ARPES. We have also shown that exciton superfluids with a p-wave symmetry condesante exhibit non trivial topological properties leading to the formation of Floquet-Majorana states.

Finally we have put developed new approximations in two extensions of DFT, namely i-DFT and ensemble DFT to study spectral properties and excited states of strongly correlated systems.

Richiesta in KE: 9 KE

ENP

Title: Exploring New Physics

Responsabile Nazionale: Giancarlo D'Ambrosio (Napoli)
Responsabile Locale: Giulia Maria de Divitiis

Anagrafica:

1) Giulia Maria de Divitiis (RU 50%)
2) Roberto Frezzotti (PA 50%)
3) Alberto Salvio(RTDB 75%)

Ricercatori 3, FTE 1.75

Attività' scientifiche:

Beyond the standard model scenarios that are valid over a vast energy range: from the Hubble up to the Planck scale. These scenarios include right-handed neutrino and an axion model. In particular, we studied dark matter and some connections with gravitational waves. New multifield model of inflation where the inflatons are a pseudo Nambu-Goldstone boson and the scalaron (the effective scalar present in Starobinsky inflation). This model is in good agreement with the recent Planck bounds.
First-principle computation in Lattice QCD of hadronic matrix elements that are relevant to constrain various possible extensions of the Standard Model -
We have worked at improving the accuracy of the theoretical predictions of leptonic decay rates through advanced lattice methods.
We have performed a high precision determination of the ratio of kaon and pion leptonic decay constants in QCD with N_f= 2+1+1 dynamical quark flavours using Wilson-clover twisted mass fermions. The simulations reach the physical pion point and include three values of the lattice spacing ranging from \sim 0.068~0.068 to \sim 0.092~0.092 fm, with linear lattice size up to L \sim 5.5L~5.5~fm. we have discussed the implications of our results for the CKM matrix element lV_{us}l and for the first-row CKM matrix unitarity.
Comparison of existing experimental data for the radiative leptonic decays $P\to\ell\nu_\ell\gamma$, where P=K or π and ℓ=e or μ, from the KLOE, PIBETA, E787, ISTRA+ and OKA collaborations against theoretical predictions based on our recent non-perturbative determinations of the structure-dependent vector and axial-vector form factors, FV and FA respectively. These were obtained for the first time using unquenched lattice QCD+QED simulations at order O(\alpha_em) in the electromagnetic coupling.
The comparison shows a good agreement with the KLOE data on $K\to e\nu_e\gamma$ decays from which the form factor F+=FV+FA can be determined. For $K\to\mu\nu_\mu\gamma$ decays instead we observe differences of up to three or four standard deviations at large photon energies between the theoretical predictions and the data from the E787, ISTRA+ and OKA experiments and similar discrepancies in some kinematical regions with the PIBETA experiment on radiative pion decays. A global study of all the kaon-decay data within the Standard Model results in a poor fit, largely because at large photon energies the KLOE and E787 data cannot be reproduced simultaneously in terms of the same form factor F+. The discrepancy between the theoretical and experimental values of the form factor F-=FV-FA is even more pronounced.
We have worked on the non-perturbative renormalization and RG-running of the Delta F = 2 four-fermion operators relevant for neutral Kaon oscillations in the SM and beyond by using the chirally-rotated Schroedinger-functional scheme. We have completed a first part of the project: the analysis of the bilinear quark currents, focusing on flavor-non-singlet pseudoscalar and tensor operators.
RESEARCH PROGRAMM 2022
Multifield models of inflation motivated by particle physics and their imprints on the relic background of gravitational waves. We will explore the possibility to distinguish between multifield and single field models of inflation through the combination of CMB observations and gravitational wave detectors.
We plan to extend the computation of the form factors for the radiative leptonic decays of pseudoscalar mesons to the case of heavy (D_s, D, B_s and B) mesons, which are challenging mainly due to technical difficulties in extracting the signal from the lowest-lying states of interest.
Dynamical generation of the electroweak scale and the universality of the physical observables in a recently proposed non-perturbative mechanism for the origin of the masses of the elementary particles from new superstrong interactions (possibly leading to a composite Higgs scenario). Here the challenge lies in the specification of the UV regulated model both from the viewpoint of its defining symmetries and in practice, i.e. upon adopting a lattice formulation suitable for first principle checks of these ideas via numerical simulation.
We plan to complete the non perturbative renormalisation of four-fermion operators involved
in neutral kaon oscillations.

Richiesta: 3 KE

QCDLAT

Title: Next generation lattice field theory for searching new phenomena in particle physics
Responsabile Nazionale: Leonardo Giusti
Responsabile Locale: Tassos Vladikas

Anagrafica:

1)Giulia Maria de Divitiis 50%
2) Mauro Lucio Papinutto 50%
3) Anastassios Vladikas 100%
4) Ludovica Pirelli 100%

Ricercatori 4, FTE 3

Attività' scientifiche:

Il nodo di Roma (ToV e RM1) dell' IS QCDLAT partecipa alle collaborazioni Alpha e CLS, concentrate nello studio della QCD con 3 sapori dinamici. Attualmente stiamo proseguendo con il completamento delle proprietà di rinormalizzazione e improvement a-la Symanzik dell' azione fermionica di Wilson e degli operatori bilineari. Avendo ottenuto buoni risultati sia per la rinormalizzazione e il RG-running della massa dl quark (quantità ZP e r_m) e il rapporto ZP/ZS delle costanti di risormalizzazione degli operatori scalare e pseudoscalare, stiamo proseguendo con i seguenti calcoli:
— rinormalizzazione ZT del operatore tensoriale T;
— coefficienti d'improvement c_A, c_V, c_T degli operatori bilineari A,V,T;
— coefficiente d'improvement b_g dell'accoppiamento dei campi di gauge.
Questi studi si effettuano nell'ambito di una formulazione mista, con fermioni di valenza con condizioni di bordo "chirally rotated Schroedinger Functional" e fermioni di mare con condizioni di bordo "Schroedinger Functional".

Una volta ottenuti questi risultati, si proseguirà alla computazione di analoghe quantità per gli operatori a 4 fermioni rilevanti alle oscillazioni di mesoni neutri in teorie BSM.

Richiesta in KE: 6.5 KE