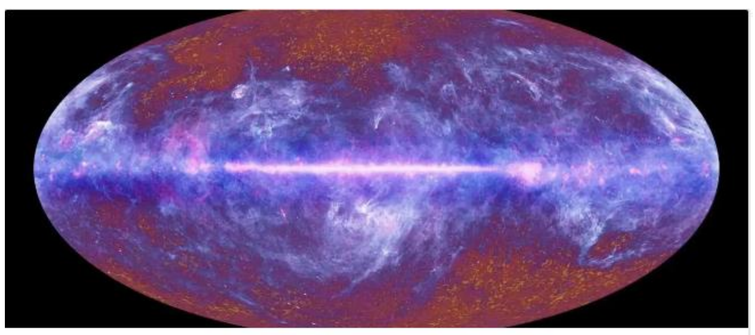
Institute for Theoretical Physics

ITFA – an overview

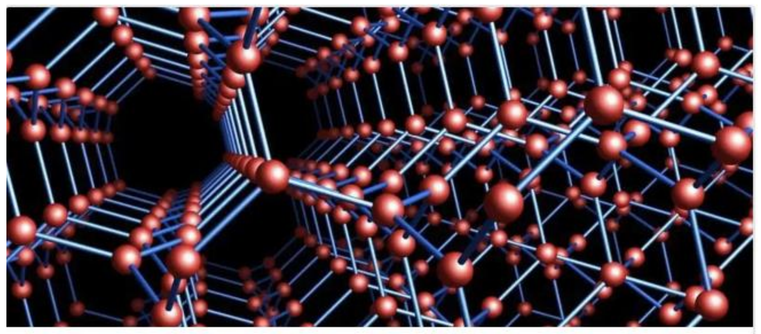
- World-leading theoretical physics institute
- What we do:
  - Astroparticle Physics (GRAPPA)
  - Condensed Matter Theory
  - Cosmology
  - History and Philosophy of Physics
  - Mathematical Physics
  - String theory
  - Theoretical particle
- Also strong links HIMS (chemistry), KdVI (maths), NIKHEF (subatomic physics), IvI (informatics)

Bachelor project philosophy

- Individual research projects, guided by faculty and doctoral/postdoctoral scientists.
- **EXPERIENCE** what the state of the art is at the research frontier.
- **LEARN** how to do research.
- **DISCOVER** - make an original research contribution!
- **COMMUNICATE** your results in both written and spoken form.
- Publish? Maybe! Some of our Bachelor projects contribute to articles in major journals.



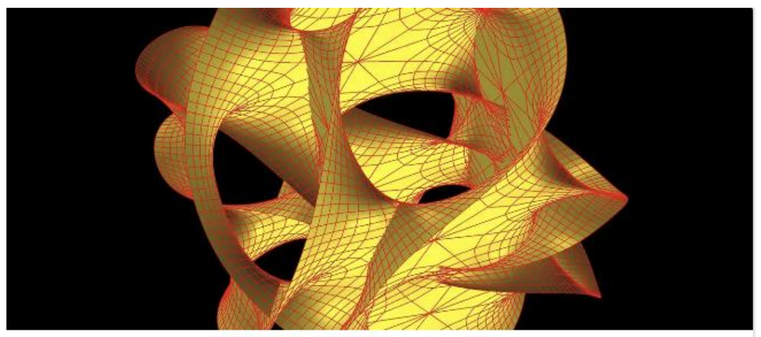
Cosmology



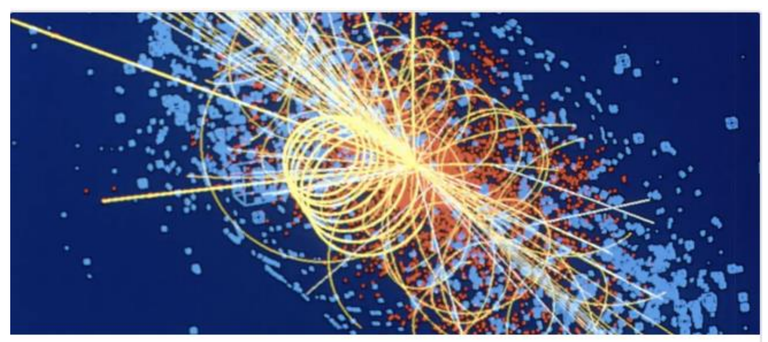
Condensed Matter Theory

GRAPPA

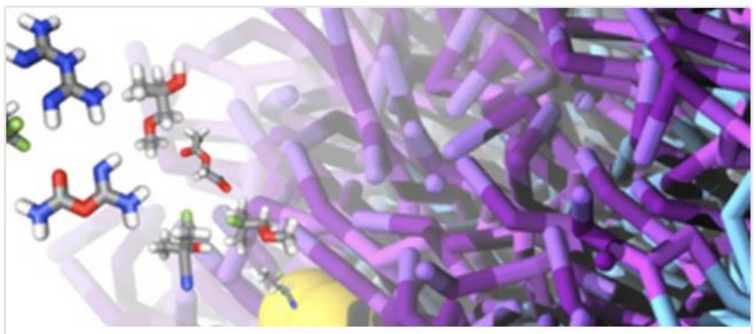
History and Philosophy of Physics



String Theory



Particle Phenomenology



Computational Soft Matter

Project types:

- Theoretical physics
- Computational physics
- Data/Statistical methods
- Mathematical methods

Next steps

- Project descriptions are on Canvas (accessible via this QR code).
- Contact the supervisor(s) directly if you are interested in a project. You can investigate several before you choose.
- Presentations are held together in a Bachelor Project Symposium).

ITFA BSc projects 2025

February 19, 2025

Topological effects in field theory: instantons and solitons
Supervisor: Dr. Wouter Waalewijn *wouterw@nikhef.nl*

Instantons are classical solutions to field equations in Euclidean spacetime, providing a framework to study phenomena like quantum tunneling. As a first step, these concepts can be explored in the context of quantum mechanics. On the other hand, solitons are classical solutions in Minkowski spacetime, representing stable, particle-like configurations. A well-known example is the magnetic monopole, which arises in certain gauge theories. In both cases, topology plays a significant role, e.g. influencing the stability of these solutions. The exact focus of the project will depend on the student's interests.

Mechanics of compressed chains of hard spheres
Supervisor: Dr. Edan Lerner *e.lerner@uva.nl*

In this project we will employ a computational framework (1) that allows to compress "pearl necklaces" — long chains of hard spheres — until they jam and cannot be further compressed. We will study these "necklace packings" and their structural and mechanical properties. In particular, we will ask how these packings differ from "plain vanilla" packings of hard spheres, the latter are known to abide by the $d \to \infty$ mean-field theory (2). This project requires some experience with coding.

(1) Edan Lerner, Gustavo Düring, and Matthieu Wyart, Simulations of driven overdamped frictionless hard spheres, Comp. Phys. Comm. 184, 628 (2013).
(2) Patrick Charbonneau, Jorge Kurchan, Giorgio Parisi, Pierfrancesco Urbani & Francesco Zamponi, Fractal free energy landscapes in structural glasses, Nature Communications 5, 3725 (2014)

Calculation of the optical absorption spectrum of real materials from an iterative Lanczos-Haydock Bethe-Salpeter method
Supervisor: Dr. Irene Aguilera *i.g.aguilerabonet@uva.nl*

The Bethe-Salpeter equation is an accurate method to calculate optical absorption spectra from first principles. These kinds of calculations do not rely on

empirical or adjustable parameters and only use the chemical composition and structure of a material as input. The Bethe-Salpeter equation can be formulated as a large eigenvalue problem. However, the solution of this eigenvalue problem can become very expensive because of the very large Hamiltonian matrix. The Lanczos-Haydock approach makes it possible to circumvent the solution of the eigenvalue problem and to calculate the optical absorption spectrum directly from the Hamiltonian in an iterative procedure. In this project, the Lanczos-Haydock method will be implemented in a Bethe-Salpeter code and its application to real materials will be tested.

First-principles calculations of the electronic structure of 2-dimensional CrI3
Supervisor: Dr. Irene Aguilera *i.g.aguilerabonet@uva.nl*

In this theoretical bachelor thesis, we will use the most popular first-principles computational method in condensed matter physics, called density functional theory (DFT), to obtain the band structures of bulk and monolayer CrI3. Monolayer CrI3 has garnered significant attention due to its exceptional magnetic and electronic properties. As one of the first 2D materials discovered to exhibit intrinsic ferromagnetism at the monolayer level, it offers unique opportunities to explore low-dimensional magnetism, spintronic applications, and the interplay between magnetism and other quantum phenomena. Beyond its ferromagnetic nature, CrI3 has been proposed to be the host of the recently predicted concept of topological magnons. This might lead to applications in spintronics, quantum information processing, magneto-optical technologies, and magnon-based computing. A computational investigation of monolayer CrI3 can provide critical insights into these phenomena and guide experimental efforts to harness its unique properties. As a long term project, my group will calculate the magnon spectra of bulk and monolayer CrI3 using other advanced first-principles methods. This bachelor thesis will be the first step in that direction. This project is embedded in the Ab Initio Quantum Materials (AIQM) group. The research will be involved in an ongoing international collaboration, which will result in a joint publication on the magnonic properties of CrI3. The results of this bachelor thesis will contribute to that publication. The theoretical simulations will be run in the Dutch supercomputer Snellius and the German supercomputer JURECA. This project is for you if you have a solid background in electromagnetism and quantum mechanics, and you are interested in numerical simulations and properties of matter.

Tensor network simulations of the spin S=2 2D Blume-Capel model
Supervisor: Dr. Philippe Corboz *p.r.corboz@uva.nl*

The Blume-Capel model is one of the simplest lattice models exhibiting a tricritical point (1). The spin S=1 case can be seen as a generalization of the well-known Ising model with additional vacancies of zero spin, whereas the spin S=2 has 5 possible states per site. The goal of this project is to study the

phase diagram of the spin S=2 model using tensor network techniques, which are a powerful class of methods to study many-body problems. The idea is to represent the partition function of the model as a 2D network of rank-4 tensors which can be efficiently evaluated using approximate contraction methods (2), where the accuracy is controlled by the so-called bond dimension of the tensors. This approach will be used to study the thermodynamic properties and phase transitions of this model in a systematic way.

(1) J. Zierenberg, N. G. Fytas, M. Weigel, W. Janke, and A. Malakis, Scaling and Universality in the Phase Diagram of the 2D Blume-Capel Model, Eur. Phys. J. Spec. Top. 226, 789 (2017). https://arxiv.org/abs/1612.02138 (and references therein)
(2) T. Nishino and K. Okunishi, Corner Transfer Matrix Renormalization Group Method, J. Phys. Soc. Jpn. 65, 891 (1996). https://arxiv.org/pdf/cond-mat/9507087.pdf

Investigation of band formation in two-dimensional systems of dipolar active Brownian particles using computer simulations.
Supervisor: Dr. Sara Jabbari-Farouji *s.jabbarifarouji@uva.nl*

Self-propelled particles with intrinsic dipole moments are naturally found in suspensions of magnetotactic bacteria or can be engineered using Janus colloids (1). Dipole-dipole interactions, which feature both long-range and anisotropic aspects, are responsible for non- reciprocal torques destabilizing the side-by-side parallel alignment of two dipoles. However, the formation of flocking collective states of motion, where particles move altogether side- by-side, was reported in a simulation investigation (2) on active Brownian dipolar particles (ABP). Interestingly, our recent numerical investigations of two-dimensional (2D) dipolar ABPs have further shown the formation of bands (see figure above) when the self-propulsion velocity exceeds a certain threshold. The formation dynamics and stability of such structures remain unclear, as purely dipolar interactions would, a priori, destabilize the horizontal alignment of dipoles. Additionally, finite-size effects in the simulated systems are believed to play an important role. In this project, you will perform Brownian dynamics simulations of 2D dipolar active Brownian particles to explore their transitions toward collective states of motion, seeking to understand the interplay between self-propulsion and dipolar interactions in the process of band formation. Comprehending the structure and dynamics of self-propelled dipolar particles is crucial for numerous innovations, such as designing smart active materials or for targeted drug-delivery applications in biomedicine. The project will involve using the high-performance computational molecular dynamics software LAMMPS and developing codes for data analysis.

(1) L. Baraban, D. Makarov, R. Streubel, I. Mönch, D. Grimm, S. Sanchez, and O.G. Schmidt.ACS Nano, 6(4):3383–3389, 2012.
(2) G.-J. Liao, C.K. Hall, and S.H.L. Klapp. Soft Matter, 16:2208–2223, 2020.

Dynamical phase transitions in active magnetic matter
Supervisor: Dr. Sara Jabbari-Farouji *s.jabbarifarouji@uva.nl*

Active magnetic systems encompass a diverse range of entities, including magnetotactic bacteria, magnetic nano- and micro-robots. The intriguing dynamics within these systems arise from the interplay between self-propulsion and the long-range dipole–dipole interactions among active magnetic particles. Notably, strong magnetic couplings prompt formation of a spanning network of particles percolates through the system at low densities, whereas at higher densities, active magnetic particles move collectively in flocking patterns with polar order. In this project you will use particle-based simulations to unravel the nature of orientational order-disorder transition at high densities.

Dynamical self-assembly of dipolar active Brownian particles in two dimensions
GJ Liao, CK Hall, SHL Klapp, Soft Matter 16 (9), 2208-2223 (2020)

Investigation of rigidity vs. Connectivity Percolation in Dipolar Active Brownian Particles using computer simulations
Supervisor: Dr. Sara Jabbari-Farouji *s.jabbarifarouji@uva.nl*

Self-propelled (active) particles with permanent magnetic dipole moments are naturally found in magnetotactic bacteria and can also be engineered in man-made systems, such as magnetic micro-robots. Brownian particles with these permanent dipole moments tend to self-assemble into chain-like structures due to long-range dipole-dipole interactions (1). When the dipole moments are sufficiently strong, these chains form a disordered network that spans the entire system, ensuring network-wide connectivity—a phenomenon known as connectivity percolation (2). This connectivity is typically accompanied by structural stability, resulting in a mechanically robust network capable of withstanding deformations, a process referred to as rigidity percolation(3). However, in systems with self-propelled particles, the activity of these particles competes with dipolar interactions, thereby reducing the average bond lifetime (4). The relationship between connectivity and rigidity percolation in dipolar particles remains an open question, particularly in active systems due to the dynamic and directional nature of dipolar interactions. It is unclear whether the rigidity transition occurs at the same dipolar coupling strengths or if higher dipolar strengths are required. In this project, you will explore connectivity and rigidity percolation transitions as functions of dipolar coupling and activity strength using Brownian dynamics simulations and mechanical deformation simulations. Gaining an understanding of the interplay between mechanical stability and network formation is crucial for designing smart materials and controlling collective properties in active matter systems. The project will involve using the high-performance computing molecular dynamics software package LAMMPS and developing codes for data analysis.

(1) Structural properties of the dipolar hard-sphere fluid at low temperatures and densities, Rovigatti, Lorenzo, John Russo, and Francesco Sciortino. " Soft Matter 8.23 (2012).
(2) Percolation on complex networks: Theory and application, Li, Ming, et al. Physics Reports 907 (2021).
(3) Rigidity Theory and Applications, Thorpe, Michael F., and Phillip M. Duxbury, eds.. Springer Science Business Media, (1999).
(4) Active string fluids and gels formed by dipolar active Brownian particles in 3D, M. Kelidou, M. Fazelzadeh, B., Parage, M. van Dijk, T. Hooijschuur, S. Jabbari-Farouji, particles, The Journal of Chemical Physics 161 (10) (2024).

Conformation and dynamics of active filaments under confinement
Supervisor: Dr. Sara Jabbari-Farouji *s.jabbarifarouji@uva.nl*

Biological filaments are ubiquitous in cells and are responsible for numerous fundamental biological processes, from replication to cell locomotion. The interplay between elastic and entropic driving forces under different confinement types such as membranous compartments or cell walls affects their structural arrangement and dynamics significantly (1). For example, confinement can promote uniform in narrow slits, but it can also introduce long-ranged disruptions of the nematic ordering field through (unavoidable) topological defects in spherical containers. However, effect of out of equilibrium active force (2) on self-organization of filaments under confinement has not been investigated. In this project, you will be performing systematic Brownian dynamics simulations of 2D semiflexible active chains (bead-spring models) of varying degrees of activity and flexibility under circular and slit confinement. You will investigate the effect of degree of confinement on the shape and dynamics of active filaments.

(1) A. Nikoubashman,The Journal of Chemical Physics 154, 090901 (2021) (2) The physics of active polymers and filaments, Roland G. Winkler and Gerhard Gompper ,J. Chem. Phys. 153, 040901 (2020)

Data-driven approach to develop active filament model for self-propelled worms
Supervisor: Dr. Sara Jabbari-Farouji *s.jabbarifarouji@uva.nl*

Recently, living worms such as T. tubifex and California blackworms have gained attention as experimental model systems for self-propelled active filaments (1,2). Early studies suggest these worms can be modeled by physically motivated active polymer models, where filaments are driven by tangential forces along their backbone, enabling self-propulsion. However, our recent findings indicate that such models capture worm dynamics only qualitatively (3). In more complex environments, data-driven models offer the potential to capture their intricate dynamics more accurately. In this internship, you will use data-driven approaches to develop more realistic models of worm dynamics, allowing for time- and space-dependent active forces as well as transverse force fluctuations. The novel

model developed through this data-driven approach can inform the design of biomimetic robotic worms with enhanced functionalities. This project involves using the high-performance molecular dynamics software Hoomd-blue , along with code development for data analysis and AI algorithms. The work will be done in collaboration with Antoine Deblais (worm dynamics) and Alberto Perez de Alba Ortiz (machine learning).

(1) A. Deblais, A. C. Maggs, D. Bonn, and S. Woutersen. Phase separation by entanglement of active polymerlike worms. Phys. Rev. Lett., 124:208006 (2020)
(2) Chantal Nguyen, Yasemin Ozkan-Aydin, Harry Tuazon, Daniel. I. Goldman, M. Saad Bhamla, and Orit Peleg. Emergent collective locomotion in an active polymer model of entangled worm blobs. Frontiers in Physics, 9:540 (2021).
(3) Locomotion of Polymerlike Worms in Porous Media R. Sinaasappel, M. Fazelzadeh, T. Hooijschuur, S. Jabbari-Farouji, and A. Deblais, arXiv:2407.18805 (2024) Contact: Dr. Sara Jabbari-Farouji (s.jabbarifarouji@uva.nl) at University of Amsterdam. You will be working in interdisciplinary computational soft matter lab (https://iop.fnwi.uva.nl/com)

Spiral charge density wave domains
Supervisor: Dr. Jasper van Wezel *van.wezel@gmail.com*

Charge density waves are spontaneous modulations of electron charge density that occur in certain types of quantum materials. Recently, it was discovered that in some of these materials, the charge order forms in domains with spiral patterns. In this project you will theoretically investigate how the spiral patterns appear and what energetic advantage allows them to be stable, as well as numerically model their evolution with temperature.

Mathematical techniques for precision experiments
Supervisor: Dr. Jordy de Vries *j.devries4@uva.nl*

Precision low-energy experiments often depend on high-precision calculations of quantum corrections to quantum mechanical potentials. Such corrections are most readily computed in momentum space but applications in nuclear/atomic/molecular systems often require a coordinate space expression. In this project, you will investigate mathematical techniques to perform the associated fourier transformations and the complications in case of singular potentials.

Integrability in quantum many-body physics
Supervisor: Dr. Vladimir Gritsev *vladgr23@gmail.com*

Description: It is well known that Yang-Baxter integrable systems have played a tremendous role both in mathematics (quantum groups, knot invariants, etc.), quantum many-body physics (lattice models, spin and electronic chains, quantum simulations) in high energy physics and string theory (QCD, AdS/CFT

correspondence, etc.). The aim of this project would be to extend the list of known integrable models and their applications.

Ergodicity-violating structures
Supervisor: Dr. Vladimir Gritsev *vladgr23@gmail.com*

Description: In recent years, we have witnessed an increasing interest in states of matter which are sort of in between the common ergodic situation and integrable (non-ergodic states). From the mathematical side some advance in understanding of these states comes from the operator algebra in the Hilbert space. The aim of this project would be to investigate (some of) these states using algebraic tools. Some relevant concepts (but not limited to) are "scars in quantum many-body systems".

Chaos in classical dynamical systems with a possible view towards quantum chaos
Supervisor: Dr. Vladimir Gritsev *vladgr23@gmail.com*

Description: First, it will be necessary to study a wide variety of classical chaotic phenomena. Second, one could in parallel compare these with quantum many- (or few-)-body quantum chaotic systems to uncover their similarities and/or differences.

GPU-accelerated magnetohydrodynamics
Supervisor: Dr. Philipp Mösta *p.moesta@uva.nl*

This project will involve porting and profiling individual computation kernels for our GPU-GRMHD code GRaM-X. GRaM-X is a dynamical-spacetime general-relativistic magnetohydrodynamics code for simulation binary neutron-star mergers and supernova explosions. The project is flexible and can be focused on performance testing and optimization of existing modules of the code for specific GPU architectures or developing new physics modules (e.g. neutrinos, equation of state, magnetic fields). The former will give the student experience working with state-of-the-art GPU systems and gain insights into modern GPU programming while the latter also involves algorithm development for computational physics in astrophysical magnetohydrodynamic simulations.

The Lorentz electron and the equivalence principle
Supervisor: Dr. Theo Nieuwenhuizen *t.m.nieuwenhuizen@uva.nl*

Lorentz in 1901 models the electron as a charged, non-spinning spherical shell in classical electrodynamics. Its Coulomb instability was counteracted when Poincaré 1905 incorporated vacuum energy with its negative pressure ("Poincaré stress"). The vacuum energy explained the "problem 4/3", the ratio of kinematic mass and electrodynamic mass. In cosmology, particle dark matter is basically ruled out, and so are modifications of Einstein gravity like Modified

Newtonian Dynamics (MOND) with its underpinnings like TeVeS and Emergent Gravity. This puts forward that "dark matter" must be a form of energy without dark matter particle. We have proposed that it is a combination of electrostatic and vacuum energy. The very same approach implies that Poincaré's idea works for arbitrary, spherically symmetric charge distribution inside the electron. It provides the long-sought derivation of the point-particle limit and an establishment of the equivalence principle without extra postulate.