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Alessandro Manacorda

# Lattice Models for Fluctuating Hydrodynamics in Granular and Active Matter

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# Lattice Models for Fluctuating Hydrodynamics in Granular and Active Matter

Doctoral Thesis accepted by
the University of Sapienza, Rome, Italy

Springer

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*A Valeria, Silvia, Giuliano e Carlo*

# Supervisor's Foreword

The Ph.D. thesis of Dr. Alessandro Manacorda deals with the theoretical foundations of hydrodynamic models for granular flows and active matter. These systems are considered among the most prominent examples of complex fluids, where the collective many-particle behavior can be surprising with respect to the simplicity of the single-particle dynamics. The work of Dr. Manacorda has been carried out at the Physics Department of the University of Rome "Sapienza" in association with the Institute for Complex Systems of the Italian Consiglio Nazionale delle Ricerche (CNR-ISC). The granular part of the thesis project was setup in collaboration with Prof. Antonio Prados of the University of Sevilla, where Dr. Manacorda has also spent a few months of his Ph.D. period.

Granular and active systems are examples of soft matter, in the broad meaning of condensed matter states where fluctuations are relevant. However, they are not relegated to the microscopic world, but can be encountered along a wide range of spatial and temporal scales. Indeed, granular matter is made of solid grains of size from tens of microns up to centimeters or even meters (as in rocks found in planetary rings), and active matter includes not only microscopic swimmers and ratchets (such as actin filaments, bacteria, sperms.) but also large groups of macroscopic animals such as fishes and birds. This brings to the fore a fundamental property of fluctuations in granular and active matter, that is, their intrinsic out-of-equilibrium nature. In both granular and active fluids, one has a flow of energy coming from some external driving device (an externally vibrated box in the granular case, some internal energy storage in the active case) which animates the system and is eventually dissipated in the environment. This energy current prevents the use of the equilibrium tools of statistical mechanics, such as the equilibrium ensembles or the free energies. Logically, the theoretical investigation of those systems needs to perform a *backward* step with respect to equilibrium statistical mechanics: We need to return to kinetic theory and work with time-dependent (and time-asymmetrical) equations for probabilities. In order to simplify the theory, we can look for some coarse-graining procedure, typically focusing on a few observables or fields which evolve *slowly* in space and time. Another crucial aspect of both granular and active fluids is their "small" size, in terms of number of elementary constituents which can be as small as a few hundreds in several physical examples. As a consequence, the amplitude of fluctuations of coarse-grained variables can be much more important than in a fluid made of $10^{20}$ molecules. The coarse-graining procedures, therefore, should include some description of fluctuations and this—in a non-equilibrium system—represents an unsolved challenge that puts the work of this thesis at the frontier of theoretical physics.

The main theoretical new results presented in this thesis, all published in peer-reviewed papers, concern the introduction of new lattice models for a granular fluid (Chaps. 4 and 5) or an active fluid (Chap. 6) and the derivation—in both cases through simplifying assumptions such as Molecular Chaos and Local Equilibrium—of continuum hydrodynamic equations with noises coherent with the microscopic probabilistic prescriptions. The derived equations, validated through comparison with numerical Monte Carlo simulations of the lattice models, have also been studied analytically in order to deduce interesting collective regimes and phases. In certain cases, the analytical study of the microscopic model has gone beyond the local equilibrium assumption, producing interesting results about spatial and temporal correlations.

My opinion is that the value of this thesis is not limited to the new results, but is enriched by the first three chapters which provide an excellent introduction to the main subjects of this investigation, that are the physics of granular matter, the physics of active matter, and the general theory of fluctuating hydrodynamics. This opening discussion takes roughly half of the length of this thesis and constitutes a complete guide for students or researchers coming from other fields. Most importantly, these first chapters offer an interesting perspective about the physical and mathematical features shared by granular and active matter, in particular with respect to their continuum (hydrodynamic) description. A unifying picture of active and granular flows is rarely considered in the literature and therefore constitutes a conceptual key point of this thesis.

Rome, Italy
April 2018

Dr. Andrea Puglisi

# Abstract

This thesis is the result of my research work as a Ph.D. student at Rome University Sapienza, under the supervision of Dr. Andrea Puglisi, and in collaboration with Dr. Antonio Lasanta, Prof. Antonio Prados and Carlos A. Plata from Sevilla University. The goal of the thesis is the formulation of the fluctuating hydrodynamics in granular and active matter by means of lattice models in the non-equilibrium framework.

The contents of the thesis are the following: Chap. 1 is an introduction to the physics of granular and active matter, where the definitions and the main phenomenology of granular and active systems are reviewed.

Chapter 2 reviews the fundamental theoretical tools for the study of granular and active systems. The formulation of kinetic theory for conservative interactions is given and later applied to the granular case, introducing some of the most important granular states. The modelization of active matter is also discussed, introducing the most important models formulated in the last years to reproduce self-propulsion and active interactions. The last section analyzes some key experiments showing a possible active behavior for driven granular systems.

Chapter 3 is dedicated to hydrodynamics. The classic formulation of hydrodynamics through the Chapman–Enskog approach is sketched and later applied to the granular case and the study of its hydrodynamical instabilities. An overview of hydrodynamics in active matter is given and compared with previous cases. Finally, the mostly studied lattice models for conservative and dissipative statistical systems are reviewed.

Chapter 4 introduces a granular lattice model to investigate the fluctuating hydrodynamics of shear modes: The hydrodynamic equations are derived from microscopic dynamics through a continuum limit. Depending on the boundary conditions, the model is able to reproduce several granular states and is predictive about their hydrodynamic instabilities.

Chapter 5 describes the properties of the granular model introduced when molecular chaos assumption is abandoned. It is shown how velocity correlations and energy fluctuations can be directly computed from microscopic dynamics,

explaining the divergence of numerical results from the uncorrelated case previously studied.

Chapter 6 introduces a lattice model of active matter. The procedure of previous chapters is used to include self-propelled particles in $d > 1$, leading to the observation of collective behavior. The linear stability of the disordered state is studied together with the fluctuations of hydrodynamic currents.

The Appendices contain the derivation of analytical results for the granular model presented in Chaps. 4 and 5 (Appendix A) and for the active model of Chap. 6 (Appendix B). Appendix C contains a list of link to videos, aimed at a novel reader to illustrate the phenomenology introduced in Part I.

Many results presented in Part II of this thesis have been already published in journal articles; the research work is here presented in a detailed and consequential manner. The interested reader can refer to:

- Chapter 4: A. Manacorda, C. A. Plata, A. Lasanta, A. Puglisi, and A. Prados. Lattice models for granular-like velocity fields: hydrodynamic description. *J. Stat. Phys.*, 164(4):810–841, Aug 2016.
- Chapter 5: C. A. Plata, A. Manacorda, A. Lasanta, A. Puglisi, and A. Prados. Lattice models for granular-like velocity fields: finite-size effects. *J. Stat. Mech. (Theor. Exp.)*, 2016(9):093203, 2016.
- Chapter 6: A. Manacorda and A. Puglisi. Lattice model to derive the fluctuating hydrodynamics of active particles with inertia. *Physical Review Letters*, 119(20):208003, 2017.

# List of Publications


[1] Alessandro Manacorda, Andrea Puglisi, and Alessandro Sarracino. Coulomb friction driving Brownian motors. *Communications in Theoretical Physics*, 62 (4):505, 2014.

[2] Antonio Lasanta, Alessandro Manacorda, Antonio Prados, and Andrea Puglisi. Fluctuating hydrodynamics and mesoscopic effects of spatial correlations in dissipative systems with conserved momentum. *New J. Phys.*, 17:083039, 2015.

[3] Alessandro Manacorda, Carlos A. Plata, Antonio Lasanta, Andrea Puglisi, and Antonio Prados. Lattice models for granular-like velocity fields: Hydrodynamic description. *J. Stat. Phys.*, 164(4):810–841, Aug 2016.

[4] C A Plata, A Manacorda, A Lasanta, A Puglisi, and A Prados. Lattice models for granular-like velocity fields: finite-size effects. *J. Stat. Mech. (Theor. Exp.)*, 2016(9):093203, 2016.

[5] A. Manacorda and A. Puglisi. Lattice model to derive the fluctuating hydrodynamics of active particles with inertia. *Phys. Rev. Lett.*, 119:208003, Nov 2017.

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While I was writing this thesis, on May 28, 2017, Francesco Totti retired from football, but his inventions and genius still inspire us today any time we need to feel brave and free. Grazie, Francesco: for the years spent watching you, for the dreams that you embodied for me and many more, for the creation of new geometries and dynamics of time and space, and for the inspiration that will last in the future.

Thanks to Nerina Marcon and Emanuela Salciccia for having been two special teachers for me, the former for inflaming my heart with the passion for science—without any rebate for the young student that I was—and the latter for the confidence and the ambition instilled since ten years ago until now.

I thank my parents, for the ceaseless love and support that allowed me to get where I am, for the goodwill and serenity that they imparted to me, giving me the possibility to live my life and make my choices, not necessarily understanding them. I thank my sister for being always my great sister, and for the many moments when she made me grow, listening to me and making me more aware.

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Rome, Italy
May 2018

Dr. Alessandro Manacorda

# Contents

# Part I
# Granular and Active Matter

# Chapter 1
# Introduction

*Like lesser birds on the four winds*
*Like silver scrapes in May*
*Now the sands become a crust*
*And most of you have gone away*

(Blue Öyster Cult)

Granular and active matter are among the most studied systems in out of equilibrium statistical physics.

The study of out of equilibrium systems is still under development and represents one of the most important progresses of statistical physics in the last century. At the end of the 19th century, equilibrium statistical physics had developed the main tools to investigate the physical properties of macroscopic systems as a statistical consequence of their macroscopic behavior. The development of the *kinetic theory* has related the time evolution and the equilibrium values of thermodynamic observables such as temperature and pressure to the microscopic dynamics of the enormous number of particles constituting the material of observation. The existence of conservation laws such as the energy conservation principle is the basis to define the tendency to *equilibrium* normally observed in gases and liquids: no matter the initial configuration of the system, the microscopic dynamics of the system leads it to a macroscopic equilibrium state with a given probability distribution of its dynamical coordinates, namely the positions and velocities of the particles of a gas, determined by the Boltzmann formula $e^{-\beta H}$ for Hamiltonian systems. The existence of an equilibrium state allows to introduce the Gibbs ensembles description and define thermodynamical functions such as the Helmoltz free energy, the entropy and so on.

 
A. Manacorda, *Lattice Models for Fluctuating Hydrodynamics in Granular and Active Matter*, Springer Theses,
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However, out of equilibrium systems are ubiquitous. First, every system at equilibrium can be driven out of it from a perturbation, inducing a heat or mass current into the system, developing spatial gradients coupled with a temporal evolution of thermodynamical quantities. This is what ceaselessly happens in *transport processes*, e.g. when a fluid is flowing under a pressure gradient or an electric current arises because of the application of a voltage. Nonequilibrium phenomena are involved in a large amount of research fields, such as climate dynamics, chemical reactions, biological physics and applications of physics to economics and social science. The basis of nonequilibrium statistical physics rely on *probability* and *stochastic processes* theory: while on one hand the huge number of microscopic components forbid any possibility of analytical computation of their motion one by one, on the other hand it allows to use limit theorems such as the Law of Large Numbers or the Central Limit Theorem, getting more precise predictions as the number of microscopic particles increase. The most ambitious goal of statistical physics is to derive the probability distribution of the microscopic variables of the considered system: if this is achieved, the computation of macroscopic observables is generally almost straightforward.

Granular and active matter are two kinds of out of equilibrium statistical systems. *Granular matter* is everything that is made of *grains*, like powders, sand, cereals, pills etc. A grain is a solid particle following the laws of classical mechanics and interacting among each other through *dissipative* collisions. The last feature is what actually makes granular matter out of equilibrium, differentiating it from colloidal particles which follow classical mechanics but undergo elastic collisions. A system can be at equilibrium if a phase-space trajectory and its time-reversed one have the same probability to occur a priori. It will be shown that dissipation makes it impossible for granular materials. Therefore, being out of equilibrium in granular matter is not the consequence of a perturbation but rather an *intrinsic* property of the physical system. This is possible because the granular description introduces a coarse-graining of the system at a mesoscopic scale, disregarding the microscopic degrees of freedom involved in collisions and absorbing the dissipated kinetic energy, restoring the energy conservation principle at a more fundamental level. Nevertheless, the description introduced has revealed to be of practical use to describe the main properties of granular materials. Research on granulars started from the observation of many unknown features in industrial devices: the observation that pressure and stress propagation followed a rather different behavior from elastic materials inaugurated a new research area, with many possible interactions with engineering problems such as the transport of grains, the mixing or separation of different kind of powders, the prevention of avalanches and the diffusion of fluids into a granular material.

*Active matter* is every system composed by many *self-propelled* units. The most natural examples are animals: their biological structure provide them the *motility*, i.e. the capability to sustain a state of motion by converting the chemical energy stored into kinetic energy. As it will be shown, the research has identified a plethora of active systems, including humans which obviously move across the space. Active matter exhibits a spectacular behavior when the units coordinate themselves and give rise to *collective motion*: this is what we observe when fishes move together in huge schools, travelling across the sea and defending from predators, or when birds coordinate their motion forming amazing flocks. Thus, active matter phenomena are the combination of the individual self-propulsion of the units with the reciprocal interactions established among them. Living units are very complex systems, and the derivation of interaction rules from their biological properties is currently out of reach. Therefore, research on active matter in the last two decades focused on the proposal of minimal models capable to reproduce the main features of collective motion observed in experiments.

Granular and active matter share two main properties:

- they are both intrinsically out of equilibrium: indeed, active matter continuously converts internal energy - absorbed somehow from the environment-in kinetic energy to sustain its state of motion; furthermore, when moving in a viscous fluid or substrate, kinetic energy is dissipated all along the motion. This implies the presence of continuous balance of energy injection/dissipation during the motion of the particle. The same balance occurs in a driven granular gas: to avoid the global "cooling" of granular motion caused by collisions, one can inject energy in a granular media through some mechanical process, like shearing or shaking the granular. Therefore, granular and active matter seem to have a *specular behavior*: while the former loses kinetic energy in its free motion and needs to absorb it from the environment, the latter vice versa "creates" kinetic energy from stored internal energy and dissipates it interacting with the environment.
- grains and active units are generally *small systems*: even if in some physical situations they can be made of $N \sim 10^5$ particles, this number is quite far from Avogadro's number $N_A \sim 10^{23}$. Therefore, the validity of limit theorems is more delicate, the *fluctuations* become relevant and can usually be compared with the magnitude of macroscopic quantities of the system. A probabilistic approach must not disregard them but rather include them in a more accurate description.

The specularity between granular and active particles is not an invention of this thesis: many studies have connected the two, and several experiments on shaken nematic or polar rods have shown their "active behavior". Actually, it is established that driven *asymmetrical* granular particles can behave as active units, because nematic or polar interactions can produce an alignment and increase of velocity correlations leading to some collective motion. Nevertheless, what has been observed numerically-and confirmed analytically in this thesis-is that dissipative granular collisions are sufficient to create velocity correlations leading a granular system to an ordered motion, even for apolar and isotropic particles.

There are several possible descriptions when looking at granular and active matter: we are interested in their *hydrodynamic description*. Namely, a granular material or an active system can be treated as a *fluid*, where each unit is analogous to a molecule of the fluid and the dynamical observables are the macroscopic fields of density, velocity and temperature, defined from classical hydrodynamic description of molecular fluids. This representation allows to recognize many collective phenomena of granular and active motion such as vortex formation, clustering, swarming and so on. Hydrodynamics is deeply related to kinetic theory, providing a statistical derivation of macroscopic observables without the need of equilibrium assumptions. Furthermore, in the last decades the theory of *fluctuating hydrodynamics* has started, aiming at reintroducing in hydrodynamic theory all the fluctuations which are typically neglected when considering systems with a huge number of particles. However, fluctuating hydrodynamics of nonequilibrium systems often relies on equilibrium assumptions; otherwise, some successful attempts of rigorous derivation for nonequilibrium systems have been done, but represent a very hard technical challenge and therefore are limited to some specific cases.

## 1.1 What is Granular Matter

Every physical system made by a large amount of macroscopic or mesoscopic particles, called *grains*, is a granular material: typical examples are sand, dust, pills, seeds, as well as iceberg groups and Saturn rings-see Fig. 1.1 [1, 2]. Granular matter is ubiquitous in everyday life: when we transport food, build houses, stock products, project industrial processes and so on. Understanding its qualities has a great importance to predict and reproduce the behavior of such materials.

Granular materials share the following properties:

- grains are *macroscopic*: they follow the laws of classical mechanics and have a large number of internal degrees of freedom, which one does not directly observe during experiments;
- grains are *solid*: they occupy a volume which is excluded to other grains during their motion;
- grains interact by means of *dissipative interactions*: because of the presence of internal degrees of freedom, after a collision the total energy of two particles is partially dissipated, mainly because of grains deformation, as heat. Therefore friction occurs at the first level of description for a granular fluid;
- the temperature doesn't affect granular dynamics, i.e. grains can always be considered at $T = 0$. Indeed, since grains are macroscopic their mechanical energy is typically many order of magnitude larger than their internal energy, namely $mv^2 \gg k_B T$ for a particle moving with velocity $v$. In kinetic theory a *granular temperature* can be introduced from statistical properties of granular motion, but it has nothing to do with room temperature.

Let us try to explain their physical meaning: since a granular material is made by many particles, statistical mechanics is the principal theoretic tool to understand its behavior. However, even if all the above-stated properties are quite general, one can see that a granular material is intrinsically different from an elastic fluid or a solid: the classic nature of grains makes the law of quantum mechanics unnecessary, and therefore the correct statistical representation must consider classic observables and interactions. Of course, each grain is made by atoms following the laws of quantum mechanics, but at this stage the grains are the "elementary particles" of our system.