Preface

The aim of the research discussed in this thesis is to make a small progress in the secular question on the nature of the glass transition. We focused, mainly with a numerical approach, on a paradigmatic glassy system, the spin glass, and we dealt with them by seeing their behavior at equilibrium as well as studying the features of their rugged energy landscape.

The equilibrium properties we were interested in concerned the universality in the glass transition and the fragility of the spin glass phase under an external magnetic field. On the side of the energy landscape, it is accepted that the energy landscape plays a major role in the slowing down of the glasses' dynamics. We tried to get a better insight by studying zero-temperature dynamics, by studying how the energy landscape becomes trivial when tuning certain parameters, and by analyzing the lowest modes of the density of states.

Scope and Organization of This Dissertation

The text is organized in four parts. In the following paragraphs we introduce briefly each of them.

Part I of this thesis is completely introductory on the systems we studied in this thesis, spin glasses. Section 1.1 aims to put the reader into context by introducing spin glasses in the frame of the glass transitions in general, by posing a historical basis about the birth of spin glasses, mentioning and explaining the development of some major theories. We get more technical in Sect. 1.2, where we detail the observables that will be analyzed throughout the rest of the text. In Sect. 1.3 we recall the reader some main concepts on scaling and renormalization group that will be useful to understand the analyses we performed.

Part II is dedicated to the study of critical properties of spin glasses through equilibrium simulations. We study the presence and the features of critical lines in the presence of perturbations on paradigmatic Hamiltonians.

In Chap. 2, which comes from Baity-Jesi et al. (J. Stat. Mech. **2014**, P05014 (2014)) and some unpublished results, we investigate, through Monte Carlo simulations with the dedicated computer Janus, whether the SG phase survives the imposition of a small external magnetic field, and thus whether there is a phase transition under the field. The two main theories on the SG phase have different predictions, so understanding whether there is or not a phase transition would be a strong factor for discrimination between the two. We find very large fluctuations in the observables we measure, and the average turns out to be a bad descriptor for our populations of measurements. Thus, we develop statistical methods and a new finite-size scaling ansatz that let us detect very different behaviors. Some of the measurements present strong signs of criticality, while others do not. It is not possible to determine which of the two behaviors will dominate in the thermodynamic limit, but we are able to set a temperature range where the would-be phase transition should be searched.

The material in Chap. 3 comes from Baity-Jesi et al. (Phys. Rev. **89**,014202 (2014)). To produce it I had the opportunity to work on large GPU clusters in Spain and in China. We did equilibrium Monte Carlo simulations on the Heisenberg spin glass with random exchange anisotropies. According to the Kawamura scenario, the chiral and the spin glass channels couple when anisotropies are introduced. We find a phase transition for each of the order parameters, and through a careful finite-size scaling analysis we conclude that the phase transition is unique. Moreover, the universal quantities we measure are compatible with the Ising universality class, instead of Heisenberg, indicating that the anisotropy is a relevant perturbation in the renormalization group sense.

Part III is on spin glasses in the absence of thermal vibration. The energy landscape appears to play a fundamental role in the sluggish dynamics that characterize a glass. It is a feature with a diverging number of dimensions, and still, it is most commonly described through a single number. This simplification is not always suitable and it is necessary to resort to different descriptors.

Chapter 4 that comes from Baity-Jesi, Parisi (Phys. Rev. B **91**, 134203 (April 2015)) is a study of the energy landscape of spin glasses as a function of the number of spin components m. When m is small the energy landscape is rugged and complex, with a large amount of local minima. An increase of m involves the gradual disappearance of most of those minima, along with a growth of the correlations and a slow down of the dynamics.

In Chap. 5, which is the result of my stay at the Center for Soft Matter Research of the New York University, we show how athermal dynamics in spin glasses is related to crackling noise, exposing the studies from Yan et al. and Baity-Jesi et al. (Phys. Rev. Lett. **114**, 247208 (2015), Range of the interactions in selforganized criticality (2015)) and unpublished material. We focus on the hysteresis of the SK model that describes spins in a fully connected graph. The dynamics along the hysteresis loop is in form of abrupt spin avalanches. We show that these avalanches cannot occur if the interactions are short-range, and that long-range interactions are a relevant perturbation to the short-range Hamiltonian. During the avalanches, furthermore, correlations between soft spins arise spontaneously, leading naturally the system to marginally stable states.

Chapter 6, based on the work of Baity-Jesi (Soft modes, localization and two-level systems in spin glasses (2015)), examines soft plastic modes of Heisenberg spin glasses in a RF, which we impose on the system in order to get rid of the soft modes due to the rotational symmetry. At low frequencies, the density of states has a non-Debye behavior, revealing the presence of a *boson peak*, a typical feature of structural glasses. These soft modes are localized, and they connect very near states, separated by very low energy barriers, which we identify as classical *two-level systems*. This helps to find a connection between the two main theories on the boson peak. On the one hand, the replica theory gives a mean field description that attributes the soft modes to a fractal energy landscape, and on the other there is the phenomenological picture of the two-level systems that attributes the excess of soft modes to a quantum tunneling between near states.

In Part IV we give our conclusions, resuming the main results chapter by chapter.

We also include several appendices. Appendix A is on Monte Carlo algorithms and on parallel computing for spin glass simulations. Appendix B is on the measurement of connected propagators in a field. Appendix C gives details on the creation of the *quantiles* defined in Chap. 2. In Appendix D we derive some identities that were crucial to make sure that our programs gave correct output. Appendix E is about error managing. Appendix F explains the energy minimization algorithms that were used in Chaps. 4 and 6.

High-Performance Computing in This Thesis

In this thesis, we present the results of several research projects on spin glasses, principally obtained through numerical simulations. Since this is a thesis in physics, we will mainly talk about the physical results, relegating to the background the numerical details.

Nevertheless, it is important to mention that extremely powerful numerical resources were necessary to arrive at some conclusions. Especially the work of Baity-Jesi et al. (J. Stat. Mech. **2014**, P05014 (2014), Phys. Rev. **89**, 014202 (2014)) would have been unthinkable with normal computing resources.

For the work of Baity-Jesi et al. (J. Stat. Mech. **2014**, P05014 (2014)), I enjoyed the chance of being part of the Janus Collaboration, a partnership of physicists and engineers that work with the (FPGA)-based machine Janus (Belletti et al., Computing in Science and Engineering **8**, 41 (2006), Yllanes Rugged Free-Energy Landscapes in Disordered Spin Systems (2011), Baños et al., Proc. Natl. Acad. Sci. USA **109**, 6452 (2012), and the recently launched *Janus II*, Baity-Jesi et al., Comp. Phys. Comm **185**, 550–559 (2014)),[1] devised expressly for Monte Carlo simulations of spin glasses. The Janus computer has been able to thermalize much larger lattices than conventional computers, at lower temperatures, and it can reach times comparable with those of the experiments done by others (Belletti et al., Phys. Rev. Lett. **101**, 157201 (2008), Alvarez et al., J. Stat. Mech. **2010**, P06026 (2010), Alvarez Baños et al., Phys. Rev. Lett. **105**, 177202 (2010), Baños et al., Proc. Natl. Acad. Sci. USA **109**, 6452 (2012)).

In the case of the work of Baity-Jesi et al. (Phys. Rev. **89**, 014202 (2014)), I was part of SCC-Computing as a member of BIFI,[2] a FP7 project that aimed at developing connections between European and Chinese scientists by giving European groups the possibility to run simulations on the supercomputer *Tianhe-1A*, which had been the most powerful machine in the world, and at the time was ranked number two in *Top 500*.[3] Only thanks to these extraordinary resources, added to a careful tuning of our simulations in order to get the maximum performance, it has been possible to obtain the results shown in this dissertation.

In addition to the aforementioned facilities, I had the chance to use the small cluster of my group in Madrid, the *Minotauro* GPU cluster in the Barcelona Supercomputing Center, the *Memento* and *Terminus* CPU clusters and some GPU for benchmarking from BIFI, and the *Mercer* cluster of the New York University.

[1] http://www.janus-computer.com/.

[2] Strategic collaboration with China on super-computing based on Tianhe-1A, supported by the EU's Seventh Framework Programme (FP7) Programme under grant agreement n°287746. http://www.scc-computing.eu.

[3] Top 500 is the annual ranking of the 500 most powerful computers in the world, in terms of flops. http://www.top500.org.

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