PHYSICS OF
MAGNETIC THIN FILMS :
THEORY AND SIMULATION

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Preface

This book is intended for graduate students and researchers who wish to understand theoretical mechanisms lying behind macroscopic properties of magnetic thin films. The book provides a full description of basic theoretical methods and techniques of simulation to help readers in their research projects.

The idea of writing this book comes from the observation of what graduate students and research beginners need for understanding theoretically properties of magnetic thin films, and for mastering fundamental theoretical and numerical techniques in their researches. Over the years, as a professor and thesis supervisor, I have seen that it is possible to master and to use various theoretical techniques by practical training on research subjects. The present book is written with this spirit in mind.

The first part of the book presents 6 chapters. Chapters 1 to 5 focus on the fundamental theory of bulk magnetic materials. Chapter 6 is devoted to the presentation of the Monte Carlo simulation methods. These chapters are part of lectures I have given during many years in a master program of physics.

The second part of the book contains eleven chapters (chapters 7 to 17), all devoted to the main purpose of the book, namely "Physics of Magnetic Thin Films: Theory and Simulation". Each chapter is devoted to a subject, written as a research paper or a review with the presentation of the state-of-the-art literature on the subject and the motivation of the chapter. A detailed description of the techniques and the presentation of the results are then shown with discussion.

For the first five chapters on the basic theory of magnetism and chapter 8, a number of exercises and problems are proposed at the end of each of these chapters for self-training. The detailed solutions are given in part III.

Two appendices, respectively on fundamental elements of statistical physics and the second quantization method, are given at the end of the book to make it self-contained.

The works used for illustrations in Part II of this book are works from the author and his doctorate students over the years. I mention at the beginning of each chapter the main references of their contributions. They all know that I am very grateful to them for uncountable wonderful moments we have spent together, and for innumerable exciting and passionate discussions we have had.

Let me summarize the contents of the chapters.

Chapter 1 is devoted to the properties of the spin, object at the heart of magnetic materials. Several properties of systems of independent spins are shown. One can mention the paramagnetism and diamagnetism observed in some materials. Spin models such as Ising, XY, Heisenberg and Potts models are introduced. Different kinds of interactions between spins are described. In particular, the exchange interaction between Heisenberg spins is microscopically calculated. This model is widely used in the subsequent chapters of the book.

Chapter 2 shows the mean-field theory applied to a variety of bulk magnetic materials such as ferromagnets, antiferromagnets and ferrimagnets. Basic notions such as the transition temperature, the heat capacity, the magnetization and the susceptibility are calculated. The mean-field theory paves the way for more sophisticated theories presented afterward.

Chapter 3 is devoted to the spin-wave theory which shows how to calculate the spin-wave spectrum and the principal thermodynamic properties of magnetic materials including ferromagnets, antiferromagnets, ferrimagnets and helimagnets. Spin waves, or magnons when quantized, are collective excitations of a system of interacting spins. Spin waves dominate thermodynamic properties of magnetic materials at low temperatures.

Chapter 4 presents the Green's function method used in magnetism. Unlike the general Green's function theory in quantum many-body problems, its version used in magnetism is simple to manipulate. It gives correct results in a wide range of temperature. It can be used to treat any kind of spin ordering, from collinear ones in ferromagnets, antiferromagnets and ferrimagnets to non-collinear orderings in helimagnets and frustrated spin systems.

Chapter 5 is devoted to the theory of phase transitions and critical phenomena in magnetic materials. Basic notions and techniques such as the renormalization group, exact methods, transfer matrix, ... are introduced here with examples. Phase transitions in thin films are in all subjects presented in part II. A familiarity with these techniques and their language is necessary to understand the remaining chapters.

Chapter 6 shows in details the Metropolis principle of Monte Carlo simulation and its implementation. Advanced techniques such as energy-histogram and multiple energy-histogram techniques, cluster-flipping methods and Wang-Landau flat energy-histogram algorithm are presented. This chapter is useful and necessary for understanding the works presented in Part II of the book.

Part II contains a number of my personal works carried out until this year on the subjects of the book. This choice of these materials was guided by the desire to show by an author the methods and techniques used to treat the subject of each chapter.

Chapter 7 is devoted to an introduction of the frustration and the presentation of a number of exactly solved models in two dimensions. These systems contain already most of the striking features of the frustration such as the high degeneracy of the ground state (GS), many phases in the GS phase diagram, the reentrance occurring near the boundaries of these phases, the disorder lines and the partial disorder. These phenomena are found in other non-solvable systems studied in the following chapters.

In chapter 8, the spin-wave theory is introduced to calculate the spectrum in ferromagnetic and antiferromagnetic thin films where the loss of translational invariance is caused by the existence of a surface or an interface. Many examples for self-training are presented.

In chapters 9 and 10, the effects of frustration in an antiferromagnetic of face-centered cubic lattice and the effects of a frustrated surface on the thermodynamic properties at finite temperatures are shown using the Heisenberg spin model and Monte Carlo simulations and the Green's function method.

Chapters 11 and 12 are devoted to the study of the spin waves in helimagnetic films in zero field and under an applied field. The surface spin configuration is calculated and the spin-wave spectrum is obtained analytically. The phase transition is studied using Monte Carlo simulation. Partial phase transitions are found in these films.

Chapter 13 shows the method to calculate the spin-wave spectrum and its effects on thermodynamic properties of a thin film with a Dzyaloshinskii-Moriya (DM) interaction. It is shown that the DM interaction affects strongly the acoustic spin waves at long wavelength.

Chapter 14 presents a study of a crystal of skyrmions generated in two dimensions using a Heisenberg Hamiltonian including the ferromagnetic interaction J, the Dzyaloshinskii-Moriya interaction D, and an applied magnetic field H. It is found that the relaxation of the skyrmion crystal is very slow and follows a stretched exponential law. The skyrmion crystal phase is shown to undergo a transition to the paramagnetic state at a finite temperature. Effects of the lattice elasticity on the skyrmion crystal is also presented.

Chapter 15 is devoted to a study of properties of a magneto-ferroelectric superlattice with a Dzyaloshinskii-Moriya interaction at the interface. It is shown that skyrmions are excited in the magnetic layers under an applied magnetic field, and they are stable up to a transition temperature. Effects of a frustration in the magnetic layer are shown to enhance the skyrmion creation.

Chapter 16 is devoted to a study of the critical exponents of magnetic thin films as a function of the film thickness. The film is studied using the ferromagnetic Ising model and the high-resolution multiple-histogram Monte Carlo technique. There is a systematic continuous deviation of the critical exponents from their 2D values. An explanation is given. For a strongly frustrated face-centered antiferromagnetic film, it is shown, using the Wang-Landau high-performance flat energy histogram, that the phase transition changes from the first order to the second order when the thickness decreases.

Chapter 17 shows how to calculate the spin resistivity in magnetically ordered materials by Monte Carlo simulations in various types of crystal: ferromagnetic, antiferromagnetic and frustrated spin systems. In simulations, various interactions are taken into account, in particular interaction between itinerant spins, interaction between lattice spins, and interaction between lattice spins and itinerant spins. A chemical potential as well as an electric field are included. To show the efficiency of the simulation method, the Monte Carlo spin resistivity as a function of temperature is compared with recent experimental data performed on semiconducting MnTe.

I would like to thank my colleagues and friends at the University of Cergy-Pontoise for their friendship and collaboration over the years. I wish to thank again my numerous former doctorate students for uncountable happy moments we have shared together in our search for the understanding of the world of physics and

beyond.

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