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978-1-107-05378-6 - Introduction to Statistical Physics and to Computer Simulations
João Paulo Casquilho and Paulo Ivo Cortez Teixeira
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Introduction to Statistical Physics

Rigorous and comprehensive, this textbook introduces undergraduate students to simulation methods in statistical physics.

The book covers a number of topics, including the thermodynamics of magnetic and electric systems; the quantum mechanical basis of magnetism; ferrimagnetism, antiferromagnetism, spin waves and magnons; liquid crystals as a non-ideal system of technological relevance; and diffusion in an external potential. It also covers hot topics such as cosmic microwave background, magnetic cooling and Bose–Einstein condensation.

The book provides an elementary introduction to simulation methods through algorithms in pseudocode for random walks, the 2d Ising model and a model liquid crystal. Any formalism is kept simple and derivations are worked out in detail to ensure the material is accessible to students from subjects other than physics.

João Paulo Casquilho is an Associate Professor at the Universidade Nova de Lisboa, Portugal. His research work includes experimental and theoretical studies in liquid crystals rheology under applied electric or magnetic fields and dynamical systems.

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J. P. Casquilho dedicates this book to the memory of his parents.
P. I. C. Teixeira dedicates this book to his parents.

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Preface

Statistical physics is a core subject in any degree course in physics, engineering physics, or physics (or chemistry) for education. Its role is on a par with that of introductory quantum mechanics: both provide an essential background in the fundamentals of physics and are prerequisites for more advanced subjects such as atomic and molecular physics, condensed matter physics or solid state physics. On the other hand, statistical physics plays a central part in laying the foundations and enabling the interpretation of classical thermodynamics, the derivation of its laws and of results for model systems such as the classical ideal gas.

Statistical physics is also an excellent vehicle for introducing numerical simulation methods, which are ever more prevalent in physics and engineering. Indeed, computer simulations in statistical physics are playing an increasingly important role in the understanding of the properties and phase transitions of physical systems. Moreover, the computational techniques of statistical physics have been fruitfully applied to problems in many other fields, such as optimisation of assembly lines in an engineering context. Monte Carlo simulations of a number of model systems are, therefore, implemented in this course.

This book grew out of a set of lecture notes for the undergraduate statistical physics course and the graduate computer simulation methods course taught by one of us (J.P.C.) to physical engineering students at the School of Science and Technology of the New University of Lisbon, Portugal (FCT/UNL), in the years 2001–2008. In its final form, the book clearly comprises too much material for a one-semester course. This enables instructors to first cover the foundations of the subject, and then make a selection of more advanced topics, on the basis of their personal preferences and those of the group being taught. This English edition is a thoroughly revised and expanded translation, by the authors, of the Portuguese edition (IST Press, Lisbon, 2011); some of the original chapters have been broken up into shorter chapters, for a sharper focus and greater clarity.

We have deliberately kept our formalism (almost) elementary; no extensive knowledge of, e.g., quantum mechanics or analytical mechanics is presupposed, which should make the book accessible to students of subjects other than physics, such as materials science, materials engineering, chemistry, chemical engineering, or biomedical engineering. A sound basis in general physics, namely classical mechanics, classical thermodynamics, electromagnetism, and some knowledge of modern physics is, however, required. We do work out most derivations in considerable detail, and provide mathematical background material in a number of appendices. Sections marked '$*$' contain more advanced material, or a more detailed discussion of, or further elaboration on, particular subjects.

This book is organised into five parts, as we now describe.

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Random walks. In the first part we give an introduction to statistical methods in physics, and to Monte Carlo simulation methods, through the study of random walks (one chapter).

Statistical thermodynamics. In the second part we present and discuss the basic postulates of statistical physics. We then develop the statistical ensemble formalism and establish the connection with thermodynamics (three chapters).

The ideal gas. In the third part we treat the classical and quantum ideal gases using the statistical ensemble formalism (two chapters). As an extension of the classical ideal gas we study the classical real gas, with a view to applications to non-ideal systems. As applications of the quantum ideal gas we discuss the free electron model in metals, Bose–Einstein condensation, thermal vibrations in crystals and blackbody radiation.

Non-ideal systems, phase transitions and critical phenomena. In the fourth part (four chapters), one chapter is devoted to the mean-field and Landau theories of magnetic phase transitions, and to spin waves. The theory and Monte Carlo simulations of the Ising model are presented in a separate chapter. There follows a chapter on liquid crystals (mostly nematic), where we discuss the analogies between mean-field and Landau-type theories of liquid crystals, and those of ferromagnetism. We introduce the Onsager theory of the nematic phase in solutions and implement Monte Carlo simulations of confined liquid crystals using the Lebwohl–Lasher model. Finally, some of the results previously obtained for phase transitions are recapitulated in the more general context of critical phenomena in a separate chapter.

Brownian motion and diffusion. In the fifth and final part (one chapter) we briefly address irreversible processes through the study of Brownian motion and diffusion, which are related phenomena. Appropriately, we start and finish this book with the random walk, as both paradigm and metaphor.

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