Quantum Theory of Magnetism

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Springer

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ISBN 978-3-540-85415-9 e-ISBN 978-3-540-85416-6
DOI 10.1007/978-3-540-85416-6
Springer Heidelberg Dordrecht London New York

Library of Congress Control Number: 2009927326

Cover design: eStudio Calamar S.L.

Printed on acid-free paper

Springer is part of Springer Science+Business Media (www.springer.com)

Preface

In the literature, theory of magnetism is available in books at two levels. At the beginners level it is dealt as a chapter in books on solid state physics. There certain basic facts about magnetism are presented and some of the theoretical ideas are mentioned almost in passing. If one wants to persue the subject in depth then one has to refer to the books at the higher level. At this level there already do exist excellent books which have either a large canvas or limit the area but go to considerable depth. These books, however, are useful to those who already are practitioners of theoretical research in magnetism and are not exactly suitable for those who want to prepare themselves for research. In other words, we find that to our knowledge, there does not exist a book on the quantum theory of magnetism which serves as a text book and also one which helps and guides one in self-study. That is, a book where every step is worked out in detail and also contains a number of problems which help in self-assessment and also which supplement the material dealt with in the text of the book. It is precisely to fill this gap, we have attempted to write this book. This need was felt by one of the authors (WN) while giving special courses to advanced students almost two decades ago. As a result he published a book with exactly the same title but in German. The book was well received and many a reader has been asking since then if there is a revised edition. As a result, the present book is an english, thoroughly revised and updated version of the original German version. The book presumes the reader to have certain basic understanding of the concepts and techniques of quantum mechanics and statistical mechanics. Except for that, the book is, we hope, self-contained in the sense that every single step has been worked out both in the main text and also in the solutions to the problems. Some of the problems have rather long solutions. Then, these represent the results which most often are assumed to be well known but in fact they need to be worked out somewhere. Some of the problems are such that the solutions impart considerable training to one who wants to start out on research and helps him in learning certain "standard" tricks in order to understand some seminal papers and also in implementing his own research programme.

The first chapter introduces, starting from Maxwell's equations, certain basic facts about magnetism such as magnetic moment, magnetization and susceptibility and also contains a section on thermodynamics as applicable to magnetic systems. If one wants to understand magnetism of materials, one has to be first clear about

the magnetism of individual atoms. This purpose is served by Chap. 2 (Atomic magnetism), in which all the important magnetic properties of atoms are discussed. We derive the electron spin and spin–orbit interaction from the relativistic Dirac equation and investigate the behaviour of an atomic electron in the field of the nucleus and also in the presence of an external magnetic field. The third chapter is devoted to "diamagnetism" which is a property possessed by *all* materials, which, however, is observable only when it is not overwhelmed by some other forms of magnetism (para-, ferro-, ferri- or antiferromagnetism). Diamagnetism in some measure can be explained as an induction effect, particularly because of the negative susceptibility. Chapter 4 deals with paramagnetism, which in contrast to diamagnetism, presumes the existence of permanent magnetic moments. These moments can either be localized stemming from partially filled electron shells of the ions in solid or they can be the moments of the quasi-freely moving band electrons. An external magnetic field tries to order them, whereas the thermal motion opposes the ordering tendency. The result is a positive susceptibility which in general is temperature dependent. Paramagnets are characterized by the fact that a direct interaction between the permanent moments, to a good approximation, can be neglected. In contrast to this, collective magetism (ferro, ferri and antiferromagnetism) is characterized by a spontaneous ordering of the magnetic moments below a critical temperature, and therefore a necessary precondition for this is the existence of a microscopic interaction between the moments. The so-called exchange interaction even though has its origin in pure electrostatic interaction cannot be understood from classical point of view. The general experience is that for a beginner this poses certain conceptual difficulties but, at the same time, it is the basis of understanding collective magnetism. Therefore exchange interaction has been discussed in considerable detail in Chap. 5. The so-called *direct* exchange interaction is determined via the overlap integrals of the wavefunctions of the participating magnetic ions. As a result it is of very short range and therefore is seldom realized in nature as compared to certain *indirect* exchange interactions which use the electrons in the conduction band (RKKY interaction) or the diamagnetic ions (superexchange, double exchange) as "catalysts" for an interaction between the localized moments. The coupling mechanisms are explained using simple cluster models and it is shown that ultimately all the interactions have the same operator form (Heisenberg model).

Having established the required conceptual basis, the last three chapters are devoted to the three important models of magnetism, namely, the Ising, the Heisenberg and the Hubbard model, respectively. In these chapters, an attempt has been made to present material such that the approach is pedagogic and at the same time gives the latest results available in literature. In doing this care is taken to derive all the results systematically and in every detail. Some of the important derivations are treated as problems whose complete solutions are given. While discussing quantum theory of magnetism it is imperative that one uses the techniques of many-body theory. In order to famialiarize the reader with these techniques, two appendices are added. The first one deals with the formalism of second quantization where all the results are worked out and to provide sufficient training to the self-learner, a set of problems is added. The second apendix is concerned with the many-body theory.

The topics in this appendix are so chosen that they are directly relevant to the theory of magnetism. Again in this appendix, too, problems are provided, some of which elucidate certain further results which are left out in the actual text.

The preperation of this book took about 3 years during which the authors were able to get together at either Berlin or Warangal for short periods, the financial support for which was provided by the Volkswagen Foundation and Kakatiya University. It is a pleasure to acknowledge the help of Dr. G. Gangadhar Reddy in various forms during the entire period of writing the book.

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July 2009

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