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(Eds.)

Quantum Magnetism

Springer

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Preface

Putting the quantum into magnetism might, at first sight, seem like stating the obvious; the exchange interactions leading to collective magnetic behavior are, after all, a pure quantum effect. Yet, for many phenomena in magnetism this underlying quantum nature may be safely ignored at least on the qualitative level. The investigation of magnetic systems where quantum effects play a dominant role and have to be accounted for in detail has, over the last decades, evolved to be a field of very active research. On the experimental side, major boosts have come from the discovery of high-temperature superconductivity in the mid-eighties and the increasing ability of solid state chemists to fashion magnetic systems of restricted dimensionality. While high-temperature superconductivity has raised the question of the link between the mechanism of superconductivity in the cuprates and spin fluctuations and magnetic order in one- and two-dimensional spin-1/2 antiferromagnets, the new magnetic materials have exhibited a wealth of new quantum phenomena of interest in their own. In one-dimensional systems, the universal paradigm of Luttinger liquid behavior has come to the center of interest; in all restricted geometries, the interplay of low dimension, competing interactions and strong quantum fluctuations generates, beyond the usual long range ordered states, a wealth of new states of condensed matter, such as valence bond solids, magnetic plateaux, spin liquid states or spin-Peierls states, to name but a few.

The idea for this book arose during a Hereaus seminar on "Quantum Magnetism: Microscopic Techniques For Novel States of Matter" back in 2002, where it was realized that a set of extensive tutorial reviews would address the needs of both postgraduate students and researchers alike and fill a longstanding gap in the literature.

The first three chapters set out to give an account of conceptual problems and insights related to classes of systems, namely one-dimensional (Mikeska and Kolezhuk), two-dimensional (Richter, Schulenburg and Honecker) and molecular (Schnack) magnets.

The following five chapters are intended to introduce to methods used in the field of quantum magnetism, both for independent reading as well as a backup for the first chapters: this includes time-honored spin wave analysis (Ivanov and Sen), exact diagonalization (Laflorencie and Poilblanc), quantum field theory (Cabra and Pujol), coupled cluster methods (Farnell and Bishop) and the Bethe ansatz (Klümper).

To close, a more unified point of view is presented in a theoretical chapter on quantum phase transitions (Sachdev) and an experimentally oriented contribution (Lemmens and Millet), putting the wealth of phenomena into the solid state physics context of spins, orbitals and lattice topology.

Aachen, Magdeburg, Liverpool, Manchester
March 2004

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1 One-Dimensional Magnetism

Hans-Jürgen Mikeska[1] and Alexei K. Kolezhuk[1,2]

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Abstract. We present an up-to-date survey of theoretical concepts and results in the field of one-dimensional magnetism and of their relevance to experiments and real materials. Main emphasis of the chapter is on quantum phenomena in models of localized spins with isotropic exchange and additional interactions from anisotropy and external magnetic fields.

Three sections deal with the main classes of model systems for 1D quantum magnetism: $S = 1/2$ chains, spin chains with $S > 1/2$, and $S = 1/2$ Heisenberg ladders. We discuss the variation of physical properties and elementary excitation spectra with a large number of model parameters such as magnetic field, anisotropy, alternation, next-nearest neighbour exchange etc. We describe the related quantum phase diagrams, which include some exotic phases of frustrated chains discovered during the last decade.

A section on modified spin chains and ladders deals in particular with models including higher-order exchange interactions (ring exchange for S=1/2 and biquadratic exchange for S=1 systems), with spin-orbital models and mixed spin (ferrimagnetic) chains.

The final section is devoted to gapped one-dimensional spin systems in high magnetic field. It describes such phenomena as magnetization plateaus and cusp singularities, the emergence of a critical phase when the excitation gap is closed by the applied field, and field-induced ordering due to weak three-dimensional coupling or anisotropy. We discuss peculiarities of the dynamical spin response in the critical and ordered phases.

1.1 Introduction

The field of low-dimensional magnetism can be traced back some 75 years ago: In 1925 Ernst Ising followed a suggestion of his academic teacher Lenz and investigated the one-dimensional (1D) version of the model which is now well known under his name [1] in an effort to provide a microscopic justification for Weiss' molecular field theory of cooperative behavior in magnets; in 1931 Hans Bethe wrote his famous paper entitled 'Zur Theorie der Metalle. I. Eigenwerte und Eigenfunktionen der linearen Atomkette' [2] describing the 'Bethe ansatz' method to find the exact quantum mechanical ground state of the antiferromagnetic Heisenberg model [3], for the 1D case. Both papers were actually not to the complete satisfaction of their authors: The 1D Ising model failed to show any spontaneous order whereas Bethe did not live up to

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the expectation expressed in the last sentence of his text: 'In einer folgenden Arbeit soll die Methode auf räumliche Gitter ausgedehnt ... werden' ('in a subsequent publication the method is to be extended to cover 3D lattices').

In spite of this not very promising beginning, the field of low-dimensional magnetism developed into one of the most active areas of today's solid state physics. For the first 40 years this was an exclusively theoretical field. Theorists were attracted by the chance to find interesting exact results without having to deal with the hopelessly complicated case of models in 3D. They succeeded in extending the solution of Ising's (classical) model to 2D (which, as Onsager showed, *did* exhibit spontaneous order) and in calculating excitation energies, correlation functions and thermal properties for the quantum mechanical 1D Heisenberg model and (some of) its anisotropic generalizations. In another line of research theorists established the intimate connection between classical models in 2D and quantum mechanical models in 1D [4,5]. An important characteristic of low-dimensional magnets is the absence of long range order in models with a continuous symmetry at any finite temperature as stated in the theorem of Mermin and Wagner [6], and sometimes even the absence of long range order in the ground state [7].

It was only around 1970 when it became clear that the one- and two-dimensional models of interest to theoretical physicists might also be relevant for real materials which could be found in nature or synthesized by ingenious crystal growers. One of the classical examples are the early neutron scattering experiments on TMMC [8]. Actually, magnets in restricted dimensions have a natural realization since they exist as real bulk crystals with, however, exchange interactions which lead to magnetic coupling much stronger in one or two spatial directions than in the remaining ones. Thus, in contrast to 2D lattices (on surfaces) and 2D electron gases (in quantum wells) low D magnets often have all the advantages of bulk materials in providing sufficient intensity for experiments investigating thermal properties (e.g. specific heat), as well as dynamic properties (in particular quantum excitations) by e.g. neutron scattering.

The interest in low-dimensional, in particular one-dimensional magnets developed into a field of its own because these materials provide a unique possibility to study ground and excited states of quantum models, possible new phases of matter and the interplay of quantum fluctuations and thermal fluctuations. In the course of three decades interest developed from classical to quantum mechanics, from linear to nonlinear excitations. From the theoretical point of view the field is extremely broad and provides a playground for a large variety of methods including exact solutions (using the Bethe ansatz and the mapping to fermion systems), quantum field theoretic approaches (conformal invariance, bosonization and the semiclassical nonlinear $\sigma-$model (NLSM)), methods of many-body theory (using e.g. Schwinger bosons and hard core bosons), perturbational approaches (in particular high order series expansions) and finally a large variety of numerical methods such as exact diagonalization (mainly using the Lanczos algorithm for the lowest eigenvalues but also full diagonalization), density matrix renormalization group (DMRG) and Quantum Monte Carlo (QMC) calculations.

The field of one-dimensional magnets is characterized by strong interactions between theoretical and experimental research: In the early eighties, the seminal papers of Faddeev and Takhtajan [9] who revealed the spinon nature of the excitation spectrum of the spin-$\frac{1}{2}$ antiferromagnetic chain, and Haldane [10] who discovered the principal difference between chains of integer and half-integer spins caused an upsurge of interest in new quasi-1D magnetic materials, which substantially advanced the corresponding technology. On the other hand, in the mid eighties, when the interest in the field seemed to go down, a new boost came from the discovery of high temperature superconductors which turned out to be intimately connected to the strong magnetic fluctuations which are possible in low D materials. At about the same time a new boost for experimental investigations came from the new energy range opened up for neutron scattering experiments by spallation sources. Further progress of material science triggered interest in spin ladders, objects staying "in between" one and two dimensions [11]. At present many of the phenomena which turned up in the last decade remain unexplained and it seems safe to say that low-dimensional magnetism will be an active area of research good for surprises in many years to come.

It is thus clear that the field of 1D magnetism is vast and developing rapidly. New phenomena are found and new materials appear at a rate which makes difficult to deliver a survey which would be to any extent complete. Our aim in this chapter will be to give the reader a proper mixture of standard results and of developing topics which could serve as an advanced introduction and stimulate further reading. We try to avoid the overlap with already existing excellent textbooks on the subject [12–14], which we recommend as complementary reading. In this chapter we will therefore review a number of issues which are characteristic for new phenomena specific for one-dimensional magnets, concentrating more on principles and a unifying picture than on details.

Although classical models played an important role in the early stage of 1D magnetism, emphasis today is (and will be in this chapter) on models where quantum effects are essential. This is also reflected on the material side: Most investigations concentrate on compounds with either Cu^{2+}-ions which realize spin-$\frac{1}{2}$ or Ni^{2+}-ions which realize spin 1. Among the spin-$\frac{1}{2}$ chain-like materials, $CuCl_2 \cdot 2NC_5H_5$ (Copperpyridinchloride = CPC) is important as the first quantum chain which was investigated experimentally [15]. Among today's best realizations of the spin-$\frac{1}{2}$ antiferromagnetic Heisenberg model we mention $KCuF_3$ and Sr_2CuO_3. Another quasi-1D spin-$\frac{1}{2}$ antiferromagnet which is widely investigated is $CuGeO_3$ since it was identified in 1992 as the first inorganic spin-Peierls material [16]. The prototype of ladder materials with spin-$\frac{1}{2}$ is $SrCu_2O_3$; generally, the SrCuO materials realize not only chains and two-leg ladders but also chains with competing interactions and ladders with more than two legs. Of particular interest is the material