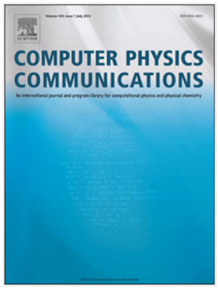
Accepted Manuscript



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PII: S0010-4655(16)30273-9
DOI: http://dx.doi.org/10.1016/j.cpc.2016.09.003
Reference: COMPHY 6044

To appear in: *Computer Physics Communications*

Received date: 4 July 2016
Accepted date: 2 September 2016

Please cite this article as: A. Hehn, N. van Well, M. Troyer, High-temperature series expansion for spin-1/2 Heisenberg models, *Computer Physics Communications* (2016), http://dx.doi.org/10.1016/j.cpc.2016.09.003

High-Temperature Series Expansion for Spin-1/2 Heisenberg Models

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Abstract

We present a high-temperature series expansion code for spin-1/2 Heisenberg models on arbitrary lattices. As an example we demonstrate how to use the application for an anisotropic triangular lattice with two independent couplings J_1 and J_2 and calculate the high-temperature series of the magnetic susceptibility and the static structure factor up to 12^{th} and 10^{th} order, respectively. We show how to extract effective coupling constants for the triangular Heisenberg model from experimental data on Cs_2CuBr_4.

Keywords: series expansions; quantum magnetism; triangular Heisenberg model

PROGRAM SUMMARY
Program Title: LCSE
Program Files doi: `http://dx.doi.org/10.17632/vygxnfjt8b.1`
Licensing provisions: Apache-2.0.
Programming language: `C++11`, MPI for parallelization, Mathematica for analysis of results.
Nature of problem: Calculation of thermodynamic properties (magnetic susceptibility and static structure factor) for quantum magnets on arbitrary lattices. A particularly hard problem pose quantum magnets on so frustrated lattice geometries, as they can not be solved efficiently by Quantum Monte Carlo methods.
Solution method: High-temperature series expansions employing a linked-cluster expansion allow to obtain a high-order series in the inverse temperature for thermodynamic quantities in the thermodynamic limit. The resulting high-temperature series are exact up to the expansion order. We implement the calculation of high-temperature series for the zero-field magnetic susceptibility and static magnetic structure factor for the spin-1/2 Heisenberg model on arbitrary infinite lattices in arbitrary dimension.
External routines/libraries: ALPS [1, 2, 3], GMP [4]

1. Introduction

Quantum antiferromagnets in low dimensions are a major topic in condensed matter physics. The initial reason for intensive study of antiferromagnetic systems was the discovery of antiferromagnetic order in the copper oxide layers of undoped parent compounds of high-temperature superconducting cuprates [5]. Since then, research on low dimensional antiferromagnetic structures has evolved into an independent field because these systems are strongly affected by quantum fluctuations and offer a great variety of exotic phases, like valence bond solids or quantum spin liquids [6]. From a theoretical perspective they are described by Heisenberg models, which are, due to their simplicity and the many exotic phases they exhibit, one of the most important class of toy models to study quantum phase transitions [7]. Furthermore, they can also serve a well controllable environment to investigate more general phenomena like Bose-Einstein condensation [8]. There exist plenty of experimental realizations for quantum magnets, such as the undoped La_2CuO_4, $NaTiO_2$ [9] or superconducting organic molecular crystals [10], to name a few. A common problem is the connection of the experiments to the theoretical models, i.e. the determination of coupling constants of theoretical models for a given material [11, 12].

An easy link between experiment and theory can be established by high-order high-temperature series expansions for the microscopic models. High-temperature series expansions have a long tradition in condensed matter physics [13, 14], and complement other numerical methods, such as exact diagonalization or quantum Monte Carlo, which are limited to small system sizes or non-frustrated systems, respectively. For translational invariant lattices, high-temperature series expansions provide results directly for the thermodynamic limit. The method is applicable to both simple bipartite spin models, as well as geometrically frustrated models or fermionic models [15] in arbitrary dimensions. The only approximation of the method is a finite order of the series.

In this paper we present a collection of applications to compute high-temperature series expansions for Heisenberg models on arbitrary lattices. As an example we compute the high-temperature series for an Heisenberg model on a triangular lattice with spatial anisotropy and show how to obtain estimates for the effective coupling constants for Cs_2CuBr_4. Previous studies of this model by Zheng et al. [16] derived the 10^{th} order series for the uniform magnetic susceptibility. We add two additional orders to this series and derived 10^{th} order series for the static magnetic structure factor.

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