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Phase diagram of the XY Vector Blume–Emery–Griffiths model on a Kagome lattice by Monte Carlo simulation

J.B. Santos-Filho [a,*], J.A. Plascak [b,c], M.C. Sobrinho [d], T.S. Araujo Batista [d]

[a] Instituto Federal de Ciências e Tecnologia de Sergipe, 49100-000 São Cristóvão, Sergipe, Brazil
[b] Universidade Federal da Paraíba, Centro de Ciências Exatas e da Natureza - Campus I, Departamento de Física - CCEN Cidade Universitária, 58051-970 - João Pessoa, Paraíba, Brazil
[c] Department of Physics and Astronomy, University of Georgia, Athens 30602 GA, USA
[d] Instituto Federal de Ciências e Tecnologia de Sergipe, 49060-108 Aracaju, Sergipe, Brazil

HIGHLIGHTS

- It treats the XY Vector Blume–Emery–Griffiths model on a Kagome lattice.
- Tricritical points or BKT endpoints and isolated critical points are present on the phase diagram for a range of model parameters.
- We compare the phase diagram with previous works and we observed that the ratio of the temperature of BKT endpoints and the BKT temperature of the pure system is a quantity independent of the lattice used.

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ABSTRACT

We present a study of the XY vectorial generalization of the Blume–Emery–Griffiths model on the Kagome lattice. Its thermodynamical properties are analyzed for different values of the Hamiltonian parameters by employing extensive and up to date Monte Carlo simulation methods consisting of hybrid algorithms. The results show a phase diagram with Berezinskii–Kosterlitz–Thouless (BKT) transitions, BKT endpoints, and isolated critical or tricritical points. We also compare the phase diagram with previous works on square and triangular lattices and we note that they are qualitatively similar. In addition, we observed that the ratio of the temperature of BKT endpoints to the corresponding BKT temperature of the pure system is a quantity almost independent of the lattice topology.

1. Introduction

The Blume–Emery–Griffiths Model [1] has been an object of intense investigations for almost five decades. It was the first discrete spin system applied to superfluidity which was able to mimic some basic features of the bulk phase diagram of ^{3}He-^{4}He mixtures. Since then, it has been used to describe various different physical systems such as metamagnetic systems, ternary alloys and fluids [2–5], among others.

Quite recently, Santos and Sá Barreto have studied the Spin-1 Blume–Capel model [6] and the Blume–Emery–Griffiths (BEG) model [7] on the Kagome lattice for different values of the Hamiltonian parameters. They have found tricritical points by employing the effective-field theory together with some rigorous bounds results. However, they were not able to study the first-order transition lines and, consequently, could not distinguish between tricritical points and critical endpoints or

* Corresponding author.
E-mail address: dr@joaobatista.eng.br (J.B. Santos-Filho).

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isolated critical points. Thus, it is important to check the existence of tricritical points, as well as other multicritical points, by using different and more powerful techniques in order to obtain the first-order transition lines.

The Kagome lattice [8] has the same coordination number of the square lattice, but different from the latter, each neighbor has another neighbor in common. Thus, the Kagome lattice, despite having the same critical exponents as the square lattice, presents different transition temperature and percolation concentration [9]. On the other hand, the Kagome lattice has been widely used in spin ice and spin liquid studies (a possible new state of matter [10–12]) because of its geometric frustration in antiferromagnetic models [13,14]. Understanding this lattice properties may therefore help to unravel new physical insights on different physical problems.

Despite the relative success in representing the physical realization of the ^{3}He-^{4}He mixtures in three dimensions, the BEG model presents a second-order phase transition in two-dimensional films, inconsistent with the experimental result of a Berezinskii–Kosterlitz–Thouless like phase transition in ^{3}He-^{4}He. This disagreement is related to the fact that the BEG model does not consider the rotational symmetry of the superfluid order parameter (or the wave function of superfluid helium). Berker and Nelson [15], and independently Cardy and Scalapino [16], proposed a planar rotator model to account for the behavior of films of ^{3}He-^{4}He mixtures, known as the vector Blume–Emery–Griffiths model (VBEG). More recently, an XY version of the VBEG model (XY-VBEG) has been treated in three dimensions where the static [17] and dynamic properties [18] have been studied through Monte Carlo and spin dynamics simulations. The XY-VBEG model is indeed a better system to describe the ^{3}He-^{4}He mixtures because it has an intrinsic dynamics, which is absent in the planar rotator version in two dimensions.

Thus, our purpose here is to study the phase diagram of the XY-VBEG model on the Kagome lattice for several values of the Hamiltonian parameters where the spins are treated as three-dimensional classical vectors. We employ a hybrid Monte Carlo algorithm in order to examine the behavior of the tricritical points and the BKT endpoints in the phase diagram. We also compare our the results obtained on the Kagome lattice with previous results on the square lattice [19] and on the triangular lattice [20].

The plan of the paper is the following. The model and the simulational methods are presented in the next section. In Section 3, we present and discuss our results, while the main conclusions are discussed in the last section.

2. Model and simulational methods

The system under investigation is an XY vectorization of the Blume–Emery–Griffiths model on a Kagome lattice. The Hamiltonian of this system can be written as

$$H = -J \sum_{\langle i,j \rangle} [S_i^x S_j^x + S_i^y S_j^y] - K \sum_{\langle i,j \rangle} S_i^2 S_j^2 + D \sum_i (S_i)^2, \tag{1}$$

where $\vec{S}_i$ represents a three-dimensional classical spin $\vec{S}_i = (S_i^x, S_i^y, S_i^z)$ with normalized magnitude $S_i^2 = (S_i^x)^2 + (S_i^y)^2 + (S_i^z)^2 = 1$ or $S_i^2 = 0$. In this case, $S_i^2 = 1$ for magnetic particles (^{4}He) and $S_i^2 = 0$ for non-magnetic particles (^{3}He). The first sum is over nearest-neighbor pairs with coupling $J > 0$, which is the term that accounts for the superfluidity. The second sum is over nearest-neighbor pairs as well, with biquadratic exchange $K > 0$. This term arises from a phenomenological modeling of the interaction energy between pairs of helium particles of the same or different species. The last sum is over all sites i of the lattice. The parameter D is a kind of crystal field, and is essentially the chemical potential difference that controls the density of non-magnetic impurities. A more detailed explanation of the above model can also be found in Ref. [17].

We consider here $J = 1$ and $K = 0$, 0.8, 1, and 1.6, and several values of the reduced crystal field variable $d = D/J$. These parameters correspond to the same values considered by Santos and Sá Barreto [7]. There are also different papers for $K = 1$ and $K = 0$ on a square lattice and on a triangular lattice for the XY version and the planar-rotator version [19–22].

The Kagome lattice was modeled using a square matrix where each element is a vector representing three sites, as described in Ref. [23]. Using this modeling the total number of sites equals to $3L^2$, where L is the linear dimension of the system.

In order to get the thermodynamic properties of the present model, we used a hybrid algorithm consisting of lattice-gas moves, combined with the spin reorientation updates. The lattice-gas update attempts to insert a magnetic particle (with a randomly selected spin orientation) at a site where a nonmagnetic one is located, or to replace the magnetic particle present at a site by a nonmagnetic one. The Monte Carlo spin updates algorithm is composed of Metropolis algorithm [24], a non-ergodic version of the Wolff algorithm [25,26] and overrelaxation updates [27,28]. The Wolff update affects only the in-plane components of the spin-1 particles, with the z-component being unchanged, in order to obey detailed balance. Analogously, the overrelaxation method is performed with a rotation solely of the in-plane component of the spins in order to keep the configurational energy fixed. The lattice-gas moves and overrelaxation are done by randomly choosing the sites of the lattice, while the Metropolis is done sequentially. The Wolff algorithm consists of flipping just one cluster. The Wolff and the overrelaxation updates are both non-ergodic, but with the spin-reorientation updates and the lattice-gas moves included, the combined algorithm will be ergodic. Each update method is performed once and each method is preceded by a lattice-gas sweep. The sequence lattice-gas–Metropolis–lattice-gas–Wolff–lattice-gas overrelaxation constitutes then one hybrid Monte Carlo step (MCS). More details can be found in Ref. [17].

For each temperature, d and K value, we have performed 5×10^5 MCS for relaxation and 5×10^5 MCS for average calculation. The phase diagram was obtained using the same methods described in the Ref [19]. First, we compare