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Monte Carlo simulation of lattice systems with RKKY interaction

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Abstract. Numerical approaches to the study of the magnetic states, properties, and phase transitions in the Ising spin systems with the long-range exchange interaction is presented. The Monte Carlo calculations have been performed for a system of Ising spins on a square lattice with long-range RKKY interaction. It is shown that the Monte Carlo simulation systems RKKY interaction leads to the formation of a complex of the magnetic structure. We compared the results of simulation with experimental images of domain structure of garnet ferrite films.

1. Introduction

Long-range interactions are rather common in nature [1]. Examples include self-gravitating systems [2], dipolar ferroelectrics, and ferromagnets in which the interactions are anisotropic with [3] RKKY interaction [4-7] and many others.

In recent years, there has been a renewed interest in Ruderman-Kittel-Kasuya-Yosida (RKKY) magnetic interaction [4-7] due to its important role in giant magnetoresistance in multilayer structures [8] and ferromagnetism in diluted magnetic semiconductors [9]. More recently, the controllable RKKY interaction attracted much attention in the field of spintronics and quantum information processing [10]. The RKKY coupling-i.e., the exchange interaction between localized core spins mediated by metallic electron gas-has been known for 50 years as the basic interaction in metallic ferromagnets. The oscillatory character of the RKKY coupling causes a spin glass behaviour in diluted magnetic metals. It rules the interlayer coupling in magnetic layered structures. As it has been shown for the last few years, the RKKY interaction is also the dominant spin interaction in diluted ferromagnetic semiconductors [9].

The lattice models have the advantage that the characteristic Hamiltonian of the system incorporates the realistic interactions between the sites and the system can be easily studied by Monte Carlo (MC) simulations [11]. Various lattice models have been introduced so far, ranging from the Ising-type models involving long range coulombian interactions [12,13] to the spin-glass type models with oscillating long range RKKY interactions [14,15].

Over the past decades, frustrated spin systems, in which all-local interactions between every spin pair cannot be satisfied simultaneously, have attracted widespread interest because very rich physics can appear in these systems [16]. The reason for this strong interest is that spin glasses exhibit a very puzzling behaviour at low temperatures, which is still not completely understood [17]. Furthermore, the theoretical treatment of these systems has led to many advances, with considerable impact on other cross-disciplinary applications such as neural networks [15] and error-correcting codes [18].

2. Approaches to simulation of a planar structure

2.1. 2-D metals

Since the presented here results concerning the 2-D arrays, it is necessary to consider a possibility of 2-D metals creation. In papers [19-21] describes the facilities of the existence in nature and the creation of real 2-D metals. According to the authors of the above manuscripts, the two main factors that have frustrated attempts to realize an "ideal" two-dimensional (2-D) metal are disorder and Coulomb repulsion. Conventional Bloch theory begins by assuming that all metals are perfect crystals and that the electrons moving through a given material only ever see the potential that is created by the ions of its crystal lattice-that is, the Coulomb interaction between electrons is negligible.

The creation of a monolayer array of superconducting niobium islands on a normal metallic gold substrate gives hope to create 2-D metals in the future [21]. The new metallic state proposed by Eley, et al. lies in a region where these pairs are mobile but are not fully Bose-Einstein condensed into a superconducting state. Such a state would be something that we have not yet encountered. Perhaps the most apt description of such a state is that of a quantum disordered phase of the condensate [21].

Based on the foregoing, it can be argued that although modern technology has not yet reached the necessity to create 2-D metal samples level, the laws of nature do not prohibit the existence of 2-D metal, so the study of the magnetic properties of such structures is necessary in fundamental and practical points of view.

In this paper we present the results of researching of properties of Ising spins on a square lattice with RKKY interaction.

2.2. RKKY interaction in superspin system

As was shown in Fischer and Klein [22], the energy of the spin system, located in the plane and interacting via RKKY exchange

$$E_{2D}(R) = -\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} A\frac{\sin x}{x^2}S_iS_j\ , \tag{1}$$

in this case $k_f^2 = 2\pi n_s$, $n_s \sim \frac{1}{a^2}$, R is the distance between particles, R_c is the radius of the sphere, a is the lattice constant-for example, for iron $a = 2.866$ Å.

2.3. The Monte Carlo simulation

In order to study frustrated spin systems, people use different computational techniques. One of these techniques is the Monte Carlo method, which is a powerful class of algorithms that is used not only in physics but also in other fields like engineering, chemistry, biology, material science, etc. [23, 24].

Although, the obtained dynamics in the Monte Carlo simulations is intrinsic and the time evolution of the system does not come from any deterministic equation for the magnetization, the results of the Monte Carlo simulations reproduce qualitatively the trend of the experimental data. Actually, this good qualitative agreement between the simulation results and the experimental data enable us to have a better insight into the nanoscale phenomena, though some of them stem from non-equilibrium processes [25].

For the simulation, we used the Metropolis algorithm [26]. The Monte Carlo (MC) simulation technique, with the implementation of the Metropolis algorithm, has been proved a very powerful tool for the systematic study of the magnetic behaviour of nanoparticles and nanoparticle assemblies.

3. Comparison of the results of numerical and physical experiments

Two well-known, well-verified complementary methods of complete enumeration and Monte Carlo simulations were used to study the state space of two-dimensional system of spins in a square lattice with long-range RKKY interaction. The purpose of these experiments was to find the configuration of

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the magnetic system corresponding to an absolute minimum of energy, calculating the degree of degeneracy of these states and checking the convergence of the results obtained by independent methods.

For systems 3x3, 4x4 were constructed phase space, see Figure 1, 2. These systems have four equally probable states with a minimum of energy.

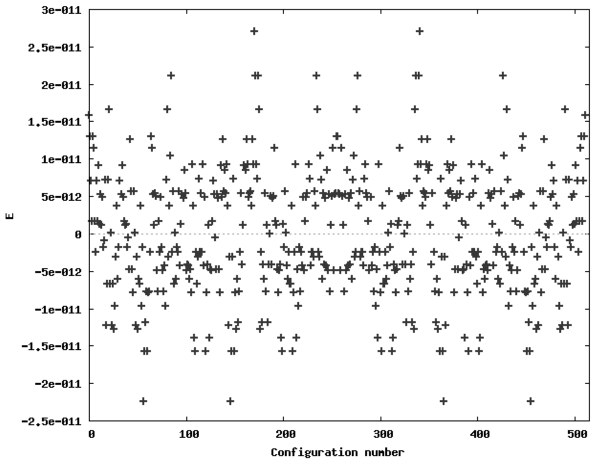

Figure 1. The phase space of system 3x3.

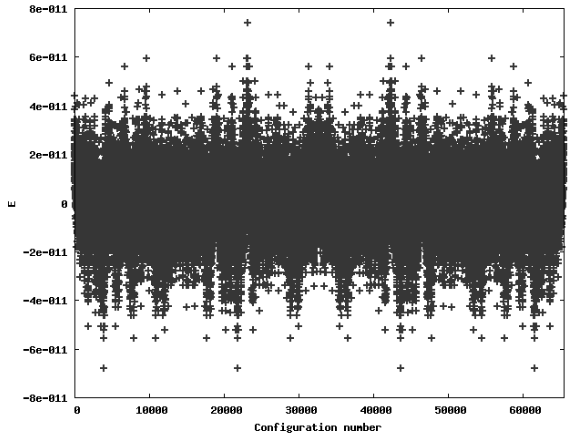

Figure 2. The phase space of system 4x4.

Monte Carlo simulations show that similar antiferromagnetic configurations of spins were observed for lattice systems with sizes up to 10x10 elements, see Figure 3. For systems, larger size observed domain structure, see Figure 4.

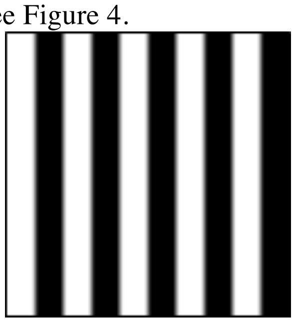

Figure 3. The system of 10x10 spins.

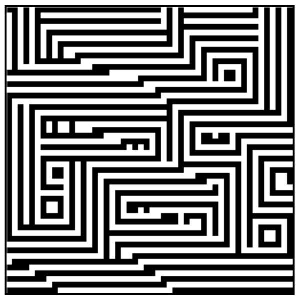

Figure 4. The system of 20x20 spins.

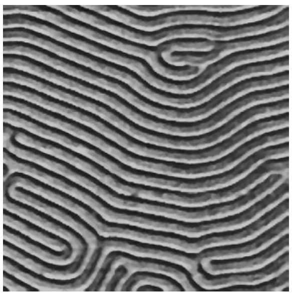

Figure 5. Size: 44x44 μm. The period of stripe domain structure is about 2 μm [27].

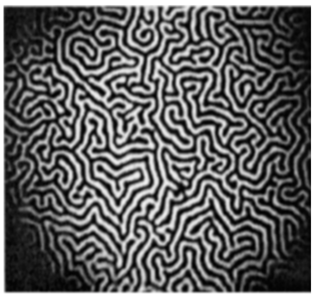

Figure 6. Dynamic domain structures [28].

Figure 5 shows experimental MFM image of the magnetic domain structure observed in the films of ferrite garnets. The film is thulium garnet iron, about 3 microns thick, is epitaxially grown on substrate of gadolinium gallium garnet [27]. Figure 6 shows dynamic domain structures was identified using the

Faraday method. In the experiment used an epitaxial (111) garnet ferrite film with the initial through labyrinth domain structure [28]. Numerical simulation of the Ising spin system with RKKY interaction by Monte Carlo method allows us to obtain the magnetic configuration of the labyrinth domain structure similar to those observed in iron-garnet films.

4. Conclusions

Monte Carlo simulation and complete enumeration in the fully connected Ising model were studied spin lattice systems with long-range indirect exchange interaction. For RKKY interacting Ising spins on a simple square lattice were studied space of states, calculated the absolute minimum of energy. Complete enumeration were investigated systems 3x3, 4x4, and 5x5, for these systems were built a phase diagram and show that there are four possible ground states. Images were obtained domain structures are presented and a qualitative comparison with experimental data was performed.

Most researchers consider that the RKKY interaction leads to frustrations and spin glass state. However, simulations shown that this interaction in the system of super-spins can lead to the formation of the domain structure, even in the absence of competition between direct of the exchange interaction and the dipole-dipole interaction.

Beyond the scope of work remained investigating, the possibility of a phase transition with Ising spin systems with direct and indirect types of exchange interaction. In the future, 3-D structures can be investigated.

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