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Monte Carlo simulation of anisotropic Shastry–Sutherland lattice in the framework of classical Heisenberg model

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Monte Carlo simulation of two-dimensional Shastry–Sutherland lattice has been carried out using heat-bath method. The dependencies of magnetization M on external field H have been obtained in the framework of classical Heisenberg model. In certain interval of exchange parameters ratio the plateau of magnetization corresponding to $M = 1/3$ has been observed. The influence of exchange anisotropy of "easy-axis" type on this plateau width is studied. It has been shown that even weak anisotropy ($\sim 1-2\%$) leads to essential enlargement of the plateau. The dependence of critical temperature on exchange parameters ratio has been established.

PACS: 75.10.Hk Classical spin models;
75.30.Gw Magnetic anisotropy;
05.50.+q Lattice theory and statistics (Ising, Potts, etc.).

Keywords: Shastry–Sutherland lattice, Monte Carlo simulation, classic Heisenberg model.

1. Introduction

Recently the physical properties of two-dimensional compounds with "Shastry–Sutherland Lattice" (SSL) magnetic structure have attracted great interest. There are many theoretical and experimental, fundamental and applied works dedicated to the given subjects. These systems are interesting due to a number of unusual magnetic properties, which exhibit various kinds of compounds. The structure of SSL can be described as a square lattice with four antiferromagnetic couplings J and one additional diagonal antiferromagnetic coupling J' [1]. It is interesting, that SSL has been considered initially by Shastry and Sutherland as an abstract model of a frustrated quantum spin system with an exact ground state in some region of parameters. Later, it has been established that a number of quasi-two-dimensional compounds have magnetic structures which are close to SSL. These are $SrCu_2(BO_3)_2$ [2–4] and rare earth tetraborides [5–7]. The experiments with these compounds have shown a number of interesting features. For example, the dependence of magnetization M on external magnetic field H contains a series of plateaux. These plateaux correspond to rational values of the ratio M/M_{sat} where M_{sat} is saturated magnetization. The plateau corresponding to $M/M_{sat} = 1/8$, $1/4$, $1/3$, $1/2$ were observed in different compounds [6–9]. As indicated above, the first measurements of magnetization peculiarities were carried out on $SrCu_2(BO_3)_2$ compound. Due to pronounced quantum magnetic properties of Cu ions, quantum SSL model were studied intensively. At the same time, such plateaux were discovered in rare-earth tetraborides RB_4 in which the rare-earth ions are placed in the (001) plane according to a lattice which is topologically equivalent to the SSL. These compounds present large total angular momenta that justify a classical description of the SSL [10–13]. Is was shown that even in classical limit and in the framework of isotropic SSL model some peculiarity on $M(H)$ dependence at $M/M_{sat} = 1/3$ takes place. This peculiarity can be identified as plateau "nucleus" (or pseudo-plateau). Spin structure corresponding to this pseudo-plateau has been established in the same paper. Later, in [12] was shown that anisotropy of exchange interaction affects the pseudo-plateau.

The main goal of our paper is to investigate in details an influence of exchange constants ratio J'/J and easy-axis anisotropy on the thermodynamic properties of two-dimensional SSL using Monte Carlo simulation in the framework of classical Heisenberg model.

2. Hamiltonian and method

The Hamiltonian of the system under consideration has the form

$$\mathcal{H} = \sum_{<i,\delta>} \mathbf{s}_i \hat{J} \mathbf{s}_{i+\delta} + \sum_{<i,\delta'>} \mathbf{s}_i \hat{J}' \mathbf{s}_{i+\delta'} - \mathbf{H} \sum_i \mathbf{s}_i . \qquad (1)$$

Here $\mathbf{s}_i$ are the classical vectors with unity length ($|\mathbf{s}_i| = 1$). Symbol $< i, \delta >$ in the first term means that the summation is taken over four near neighbours and $< i, \delta' >$ in the second term means the summation with one diagonal neighbour. The last term is the interaction of the spins system with the external magnetic field $\mathbf{H}$. The elements of diagonal matrixes

$$\hat{J} = \begin{pmatrix} J_{xx} & 0 & 0 \\ 0 & J_{yy} & 0 \\ 0 & 0 & J_{zz} \end{pmatrix}$$

and

$$\hat{J}' = \begin{pmatrix} J'_{xx} & 0 & 0 \\ 0 & J'_{yy} & 0 \\ 0 & 0 & J'_{zz} \end{pmatrix}$$

are the exchange constants ($J_{\alpha,\alpha} > 0, \alpha = x, y, z$).

A number of interesting features has been discovered in SSL in the framework of classical Monte Carlo method with Metropolis test. It should be noted that along with evident advantages (simplicity and universality) the method possess a number of disadvantages. The most important of them is low efficiency in low-temperature region. It is essentially because the specific characteristics of SSL manifest itself in full measure just in this temperature region. Further, low efficiency of the method leads to limitation on the system size (as far as we know, the maximal system size studied in the previous works is about 40×40). As the result the question about an influence of boundary effects is open yet. In this work we propose algorithm of Monte Carlo simulation based on the so-called "heat-bath" method. The method significantly improves computing efficiency at low-temperatures region and for systems with continuous degrees of freedom. Moreover, we adopted the method for parallel (cluster) calculations, which allows us to improve the efficiency also.

In the framework of "heat-bath" method the transition probability from "old" configuration s to a "new" one s' has the form [14]

$$w(s, s') = \frac{f_a(s, s')}{\sum_{\{s'\}} f_a(s, s')} . \qquad (2)$$

Symbol $\{s'\}$ means summation over all possible states of spin s'. For our calculation the acceptance probability f_a has been chosen in Metropolis form:

$$f_a(s, s') = \exp(-\beta [E(s') - E(s)])$$

where $\beta = 1/T$ is inverse temperature (T is in energy units) and $E(s)$ is the system energy in configuration s. In such a case (2) depends on s' only and acquires the form

$$w(s, s') = \frac{\exp(-\beta E(s'))}{\sum_{\{s'\}} \exp(-\beta E(s'))} . \qquad (3)$$

According to Monte Carlo approach the configurations s and s' differ by the state of one particle which we will indicate by index i. Let us introduce

$$\mathbf{S}_i = \sum_{\delta} \hat{J} \mathbf{s}_{i+\delta} + \hat{J}' \mathbf{s}_{i+\delta'} - \mathbf{H} . \qquad (4)$$

Then

$$E(s') = E(\mathbf{s}_i) = \sum_{\delta} \mathbf{s}_i \hat{J} \mathbf{s}_{i+\delta} + \mathbf{s}_i \hat{J}' \mathbf{s}_{i+\delta'} - \mathbf{H} \mathbf{s}_i = \mathbf{s}_i \mathbf{S}_i \qquad (5)$$

and

$$w(s, s') = w(S_i, \xi) = \frac{\exp(-\beta E(\mathbf{s}_i))}{Z_i} = \frac{\exp(-\beta \mathbf{s}_i \mathbf{S}_i)}{Z_i} = \frac{\exp(\xi S_i)}{Z_i} . \qquad (6)$$

Here $S_i = \beta |\mathbf{S}_i|$ and $\xi = \cos(\pi - \theta)$, where θ is the angle between $\mathbf{s}_i$ and $\mathbf{S}_i$. This choice of ξ is determined by antiferromagnetic interaction among the spins. Z_i is normalization constant in denominator (3). In our case

$$Z_i = \int_{-1}^{1} \exp(\xi S_i)\, d\xi = \frac{2}{S_i} \sinh(S_i) . \qquad (7)$$

Thus,

$$w(S_i, \xi) = \frac{S_i}{2 \sinh(S_i)} \exp(\xi S_i) . \qquad (8)$$

Performing non-linear white noise selection

$$\gamma(\xi) = \int_{-1}^{\xi} w(S_i, \xi) d\xi' = \frac{\exp(\xi S_i) - \exp(S_i)}{2 \sinh(S_i)} \qquad (9)$$

we obtain finally

$$\xi^r = \cos(\pi - \theta) = = \frac{1}{S_i} \ln \Big(\exp(S_i) - \gamma_0^r [\exp(S_i) - \exp(-S_i)] \Big) \qquad (10)$$

where γ_0^r is uniformly distributed random number ($0 \le \gamma_0^r < 1$). This expression has the following sense. Let us introduce local polar coordinate system with $z_{\|} - \mathbf{S}_i$ and arbitrary direction of x and y in the plane perpendicular to z. In such a case (10) gives the transition probability of spin $\mathbf{s}_i$ to a new state as the function of polar angle θ. As far as (5) depends on θ only one can choice azimuthal angle ϕ in xy plane as $\phi = 2\pi\gamma_1^r$, where γ_1^r is uniformly distributed random number ($0 \le \gamma_1^r < 1$).

Performing back transformation to global Cartesian coordinate system we obtain

$$\mathbf{s}_i = \begin{cases} x = n_z \sqrt{\dfrac{1-(\xi^r)^2}{l_1}} \cos(\phi) \\ y = n_z \sqrt{\dfrac{1-(\xi^r)^2}{l_2}} \sin(\phi) \\ z = (\xi^r - n_x x - n_y y)/n_z \end{cases} \qquad (11)$$

where

$$\mathbf{n} = \frac{\mathbf{S}_i}{|\mathbf{S}_i|} = \{n_x, n_y, n_z\},$$

$$l_1 = a\cos^2(\phi_0) + b\sin^2(\phi_0) - c\sin(\phi_0)\cos(\phi_0),$$

$$l_2 = a\sin^2(\phi_0) + b\cos^2(\phi_0) + c\sin(\phi_0)\cos(\phi_0),$$

$$a = n_x^2 + n_z^2,\ b = n_y^2 + n_y^2,\ c = n_x n_y,\ \phi_0 = \arctan\left(\frac{c}{b-a}\right).$$

The final expression (11) describes the probability of system transition as the function of uniformly distributed random numbers γ_0^r and γ_1^r. This Monte Carlo algorithm was tested on exact solvable models. Beside this, the search algorithm for the configurations corresponding to a minimum of internal energy is realised. The analysis of the properties of such configurations is extremely important for studying the ground state structure.

3. Results and discussion

One of the SSL distinctive features is a step-like behavior in the field dependence of magnetization M. Such behavior takes place even in the case of isotropic spin–spin exchange interaction. In the framework of classic Heisenberg model the plateau takes place for $M = 1/3$ [11] (as far as $M_{\text{sat}} = 1$ here and further more $M/M_{\text{sat}} = M$). The dependence $M(H)$ obtained in the framework of our approach for isotropic case and $\mathbf{H} \| z$ is presented in Fig. 1,*a*. Here $J_{xx} = J_{yy} = J_{zz} = 1$, $J'_{xx} = J'_{yy} = J'_{zz} = 2$, temperature $T = 0.02$ and system size is 48×48. It should be stressed, that our result is in good agreement with literature data [11,12].

On the first stage of our investigation we have studied influence of exchange anisotropy on such a peculiarity. Corresponding dependence for the case of exchange anisotropy is presented in Fig. 1,*b*. Here $J_{xx} = J_{yy} = 1$, $J'_{xx} = J'_{yy} = 2$ $J_{zz} = 1+\alpha$, $J'_{zz} = 2J_{zz}$ and anisotropy parameter $\alpha = 0.05$. One can see that even weak anisotropy ($\alpha \sim$ 5%) leads to essential growth of "step", corresponding to $M = 1/3$ [12]. Another important thing is that the curves corresponding to different system sizes (24×24 and 48×48) are in a good agreement. It means that boundary effects are small and, thus, such system size is appropriate for our calculations. The dependence of $M = 1/3$ magnetization plateau width, Δ, on α is presented in Fig. 2. It should be noted that increase in α leads to Δ growth only. The plateaux corresponding to $M \neq 1/3$ are absent.

Spin configurations corresponding for $M = 1/3$ phase coincide with those ones described in [11]. The calculated data (solid boxed) have been fitted by power function $\Delta = A\alpha^{1/k}$. The best fit corresponds to $A = 0.36$ and $k = 1.73$ which is very close to $\sqrt{3}$.

On the second stage we have determined the region of the step-like peculiarity as the function of exchange constants ratio $\mu = J'/J$. The dependence of plateau width Δ on μ for $\alpha = 0.005$ is presented in Fig. 3. One can see that in the phase, corresponding to $M = 1/3$ plateau exists in the region $1.5 \lesssim \mu \lesssim 2.4$.

On the next stage we have studied temperature dependencies of specific heat

$$C(T) = \frac{1}{T^2}(<E^2> - <E>^2)$$

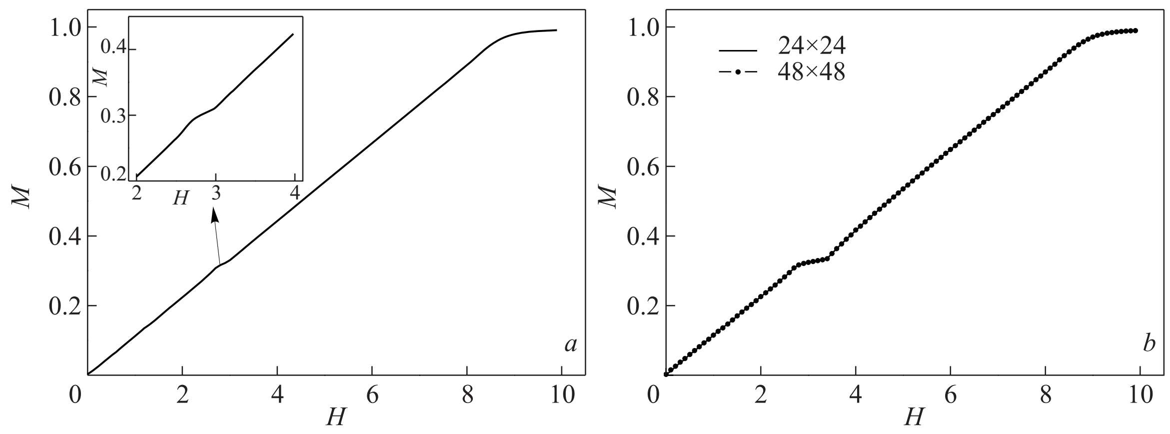

Fig. 1. The dependence of magnetization *M* on external magnetic field *H* for system size 24×24, $\mu = J'/J = 2$ and anisotropy parameter $\alpha = 0$ (isotropic case). The vicinity of pseudo-plateau $M = 1/3$ are presented in the inset (*a*). The same dependence for $\alpha = 0.05$. The temperature $T = 0.02$ was used for both figures (*b*).

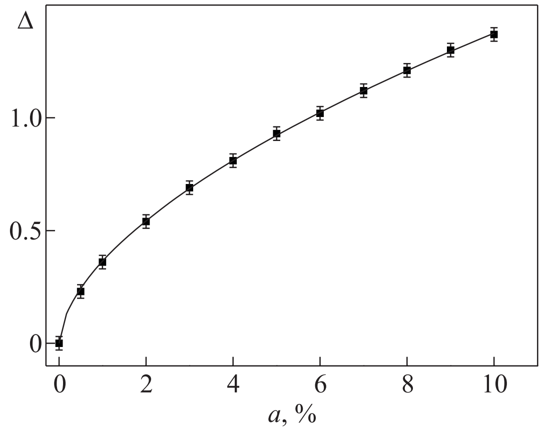

Fig. 2. The dependence of plateau width Δ on anisotropy parameter α for system size 24×24, $\mu = J'/J = 2$, $H = 0$ and $T = 0.02$.

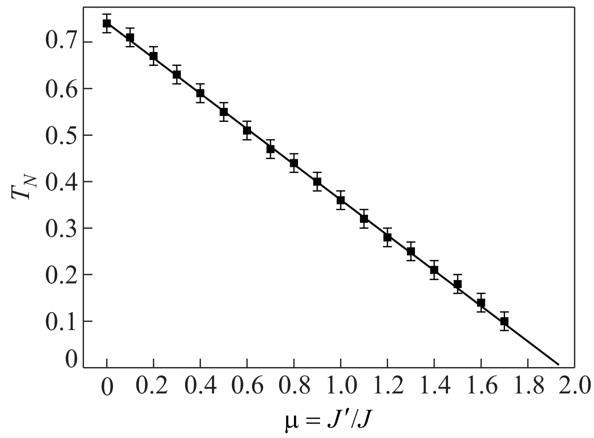

Fig. 4. The dependence of critical temperature T_N on exchange constants ratio μ for system size 24×24, $H = 0$, and $\alpha = 0$ (isotropic case). Solid boxes are calculated values, solid line is fitting by linear function.

and magnetic susceptibility

$$\chi(T) = \frac{1}{T}(< M^2 > - < M >^2).$$

Here $< E >$ and $< E^2 >$ are average energy and square average energy, respectively. These averages have been calculated also in Monte Carlo process. It is well known that these quantities are the most sensitive for the phase transitions in antiferromagnetic compounds. Analysing these curves for different μ values one can plot the dependence of critical temperature T_N on μ (Fig. 4). As seen from this figure, T_N goes to zero for $\mu \to \mu_0 \approx 1.96$. It should be noted, that μ_0 is very close to critical point value for classical SSL model ($\mu = 2$) [11]. Another interesting thing is applicability of Mermin–Wagner theorem for the system under consideration. Really, according to Mermin–Wagner theorem continuous symmetries cannot be spontaneously broken at finite temperature in isotropic two-dimensional systems with sufficiently short-range interaction. In real systems there are many reasons resulting in Mermin–Wagner theorem violation. This is quasi-two-dimensionality, long-range interaction etc. In numerical experiments this is, for example, pseudo random distribution of random number. The correlation length is large, but finite. Another important reason is discreteness of real number representation in computer. The density of numbers is not constant. In our case it leads to appearance of extremely small, but finite effective anisotropy. In addition, if long-range correlations decay slow, then it is very difficult to detect this phenomena numerically (including Monte Carlo method). It is necessary to consider extremely large systems and calculation time becomes huge. Even so, boundary effects can be small, but boundary conditions can affect on correlation functions behavior. The detailed discussion dedicated to Mermin–Wagner theorem applicability for SSL model goes beyond the scope of this paper. We plan to investigate this problem in near future.

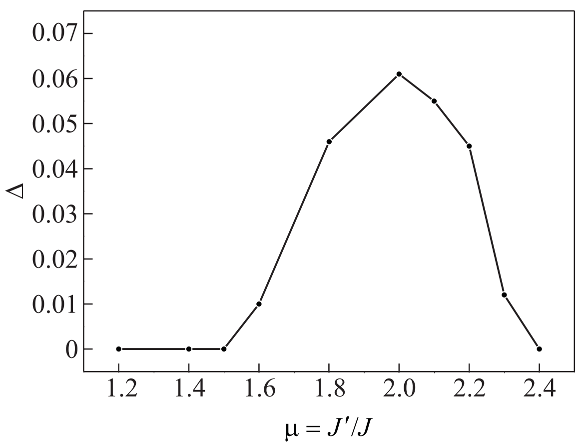

Fig. 3. The dependence of plateau width Δ on exchange constants ratio μ for $\alpha = 0.005$, system size 24×24, $H = 0$ and $T = 0.02$.

Unlike experimental data, any low-temperature (below T_N) peculiarities of $\chi(T)$ and $C(T)$ are absent in the framework on the proposed classical model. It confirms indirectly that the unusual low-temperature behavior of $\chi(T)$ inherent in SSL has quantum origin.

In addition, in order to check our results we have carried out a number of computer simulation using multicanonical method, described in [15,16]. We have extended this approach to the systems with continues degrees of freedom. It should be noted that the results obtained in the framework of both Monte Carlo methods are in good agreement.

4. Conclusions

We have studied numerically two-dimensional Shastry–Sutherland lattice in the framework of classical Heisenberg model. Parallel Monte Carlo algorithm based on heat-bath method has been developed. It has been shown, that the influence of boundary effects on SSL magnetic properties is extremely small for the systems with sizes greater than 24×24. The dependence of magnetization plateau width Δ on anisotropy parameter α has been established. This dependence can be approximated well by power function

$$\Delta = A\alpha^{1/\sqrt{3}}.$$

The plateau corresponding to $M \neq 1/3$ are absent in the framework of this classical model. It has been determined that critical temperature T_N depends linearly on exchange constants ratio μ. The extrapolation of $T_N(\mu)$ shows that the critical temperature goes to zero for $\mu \to \mu_0 \approx 1.96$. The obtained limiting value μ_0 is very close to critical point for classical SSL model ($\mu = 2$).

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