Creation and Stability of Skyrmion State in Two-Dimensional Magnets at Doping

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Abstract

It was shown that the hole introduced in CuO_2 plane causes the creation of the skyrmion spin configuration. The stability of the skyrmion state is investigated. It was established that the critical values of the exchange interaction anisotropy and interaction between planes at which skyrmion starts to destroy, are much more than in real cuprates.

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The discovery of high-temperature superconductors has led to numerous theoretical and experimental efforts to understand magnetic and electrical properties of these compounds. The most of works, in which the behaviour of superconductors was studied, consider the mobility of current carriers appearing with doping of parent compounds by Sr^{2+} ions, while smaller attention was given to the transformation of magnetic properties.

However, there is a number of works, in which the occurrence or distortion of antiferromagnetic order caused by the hole is investigated. Shraimann and Siggia [1] considered the distortion of spin ordering of spiral type induced by a hole. Gooding [2] and Morinari [3] showed that an electronic hole, introduced in the CuO_2 plane, leads to the creation of a skyrmion. In this work we propose our study of spin configuration appearing in a two-dimensional magnet with doping.

We start with the equation of motion for the magnetic moment:

$$\frac{\partial \vec{M}(\vec{r},t)}{\partial t} = g(\vec{M}(\vec{r},t) \times \vec{h}(\vec{r},t)) + \vec{R}(\vec{r},t), \tag{1}$$

where $\vec{h}(\vec{r},t)$ is an effective magnetic field of other magnetic moments, which affects on magnetic moment $\vec{M}(\vec{r},t)$, $\vec{R}(\vec{r},t)$ is a relaxation term. The first term in (1) describes the magnetic moment precession in a local magnetic field, the second one describes the relaxation to the equilibrium configuration as a result of dissipation of energy. In general the form of the relaxation term was obtained [4] from the energy conservation law:

$$\vec{R}(\vec{r},t) = \frac{1}{\tau_1}\vec{h}(\vec{r},t) - \frac{1}{\tau_2}(\vec{n}(\vec{r},t) \times (n(\vec{r},t) \times \vec{h}(\vec{r},t))), \tag{2}$$

where $\vec{n}(\vec{r},t) = \frac{\vec{M}(\vec{r},t)}{|\vec{M}(\vec{r},t)|}$; τ_1, τ_2 are constants. First term in (2) describes relaxation of magnetic moment $\vec{M}(\vec{r},t)$ magnitude, the second one describes the relaxation of magnetic moment direction to the easy magnetization axis that is determined by the direction of $\vec{h}(\vec{r},t)$.

In the case of a two-dimensional Heisenberg magnet it is possible to proceed from the magnetic moment density $\vec{M}(\vec{r},t)$ to the spin $\vec{s}(i,k)_t$ in a discrete lattice, where (i,k) are indexes, which determine the position of spin in the lattice. In the exchange-constrained spin system the local field can be obtained on the basis of the quantum mechanical equation of motion for the spin $\vec{s}(i,k)_t$ with exchange interaction Hamiltonian:

$$i\frac{\partial \vec{s}(i,k)_t}{\partial t} = [H_{s-s}(t), \vec{s}(i,k)_t] = i(\vec{s}(i,k)_t \times \vec{h}(i,k)_t) \tag{3}$$

Calculation of the commutator $[H_{s-s}(t), \vec{s}(i,k)_t]$ gives the expression for $\vec{h}(i,k)_t$:

$$\vec{h}(i,k)_t = J\sum_{\delta} \vec{s}(i+\delta, k+\delta)_t, \tag{4}$$

where J is the nearest-neighbors exchange coupling constant, δ connects nearest neighbors.

The method of the equilibrium configuration search was developed by Waldner [5]. In the expression (2) $\tau_2 \ll \tau_1$; it means that the turn of the magnetic moment towards the easy magnetization axis happens much faster than the magnitude of the magnetic moment reaches its equilibrium value.

The relaxation of the spin system to the state with minimal energy can be described as follows: after the initial state definition the iteration process starts and during this iteration process spin $\vec{s}(i,k)$ changes its orientation:

$$\vec{s}_{j+1}(i,k) = \vec{s}_j(i,k) + \Delta\vec{s}_j(i,k), \tag{5}$$

where j numbers a step of iteration. $\Delta\vec{s}(i,k)$ by analogy with the second term in (3) has a following form:

$$\Delta\vec{s}_j(i,k) = \left(\vec{s}_j(i,k) \times \vec{h}_j(i,k)\right) \times \vec{s}_j(i,k). \tag{6}$$

Thus, during the relaxation procedure, the change of spin direction $\Delta\vec{s}(i,k)$ is calculated, and then the spin $\vec{s}(i,k)$ normalizes to the unity. This iteration procedure is continued until $\Delta\vec{s}(i,k)$ became sufficiently small (less than some precision ε).

Now we define the initial state with condition that the full magnetization equals to zero (the Mermin-Wagner-Hohenberg theorem). At first we consider a more simple case of ferromagnet of $m \times m$ spins. We set the spin configuration in the form of four domains, each of which has a uniform magnetization. Domains are separated by the domain walls in such a way that the full magnetization of the spin lattice is equal to zero (See Fig.1).

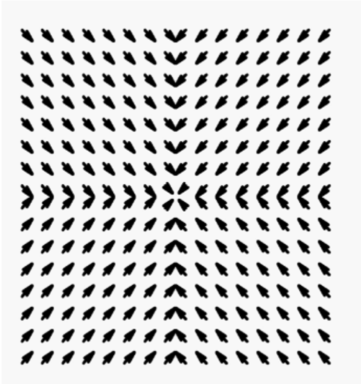

Figure 1: The initial state. Projection on the $0xy$ plane. Ferromagnet. The lattice of 16×16 spins.

Then we consider how the spin configuration changes with doping. We suppose that in the sample many holes were introduced and that they have periodic distribution. According to the work of Gooding [3], the hole moves over the four oxygen ions, which are between the copper ions. It leads to the distortion of the copper ions spins orientation. Therefore we assume that the z-component of the four copper ions spins near the hole became non-zero, while all other spins lie in the plane. This state is unstable. Then we find equilibrium spin configuration using the method described above.

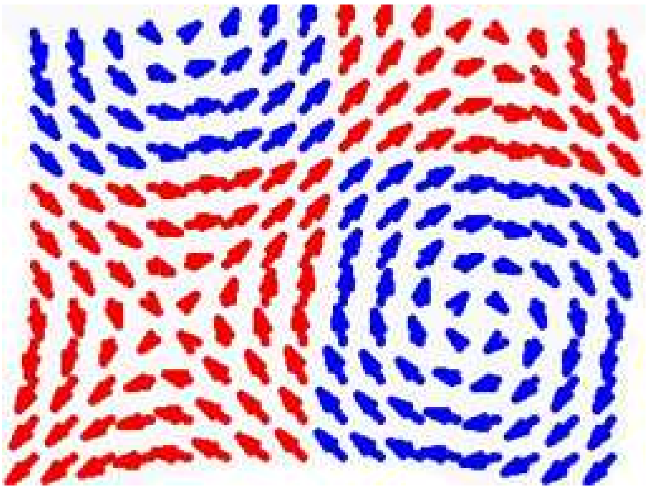

Figure 2: The periodic structure of skyrmions and antiskyrmions. Projection on the $0xy$-plane. Ferromagnet. Spins, directed upwards, are blue; spins, directed downwards, are red.

After the procedure of relaxation spin system reaches its equilibrium state. The projection of spins on $0xy$-plane is shown in Fig.2, three-dimensional distribution of z-component is shown in Fig.3. As can be seen from Fig.2, Fig.3 periodic lattice of skyrmions and antiskyrmions is formed in the sample.

Then we consider the case of antiferromagnet. It was established that in antiferromagnet at doping the electronic holes leads to the formation of the skyrmions and antiskyrmions system in two sublattices (See Fig.4). It confirms the validity of Gooding assumption that the quasilocal movement of the hole introduced in CuO_2 plane causes the creation of the skyrmion. In the following study of the skyrmion state stability we consider the case of ferromagnet for the simplicity.

Now the question of stability of the skyrmion state at the transition from ideal two-dimensional Heisenberg magnet to the real cuprates is arisen. We consider the influence of the exchange interaction anisotropy and the interaction between planes on the form, size and, in general, existence of skyrmions.

It was found, that the form of skyrmion essentially changes depending on a value of the exchange interaction anisotropy. In Fig.5 the crossection of the spin configuration by the $0xz$-plane is shown. As can be seen, in the case $J_z > J_{x,y}$, even at small difference between components of the exchange coupling constant ($J_{x,y} \leq J_z \leq 1.02 J_{x,y}$) the skyrmion state still takes place, but its form begins to distort. When $J_z \geq 1.02 J_{x,y}$ skyrmions disappear and the domain structure, reminding initial, is formed. In the case

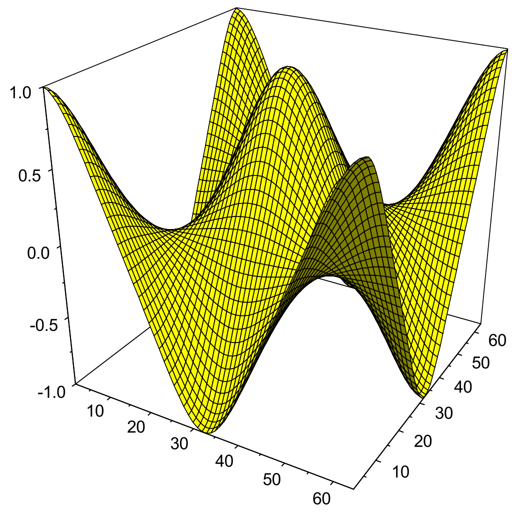

Figure 3: The periodic structure of skyrmions and antiskyrmions. z-component. Ferromagnet.

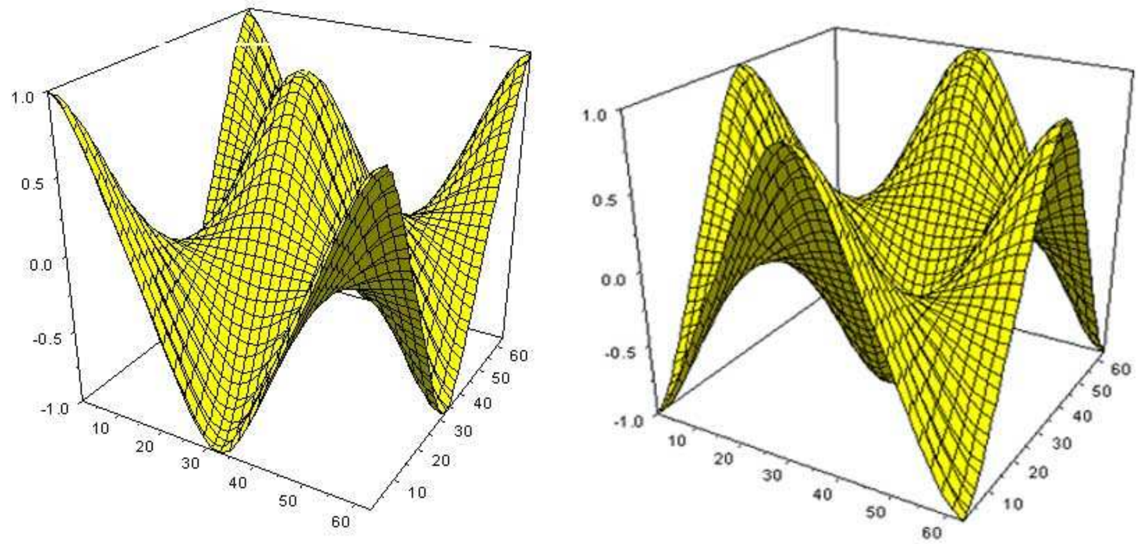

Figure 4: The periodic structure of skyrmions and antiskyrmions. z-component. AntiFerromagnet. Two sublattices.

$J_z < J_{x,y}$, skyrmion tends to lie on the plane and to turn into the two-dimensional vortex. At $J_z \leq 0.7J_{x,y}$ periodic structure of vortexes is arisen.

When we took into account the interaction between planes two cases were considered: two weakly-interacted planes (like in $YBa_2Cu_3O_6$ with antiferromagnetic coupling between planes) and completely three-dimensional case (the cube of $m \times m \times m$ spins) with the weak exchange between planes (like in La_2CuO_4 with antiferromagnetic coupling between planes too).

It was established that in the case of two weakly-interacted planes skyrmion is destroyed by ferromagnetic coupling between planes of order $J_1 = 0.03J$ (where J is in-plane exchange coupling constant) and antiferromagnetic coupling $J_1 = -0.09J$. In the three-dimensional case the skyrmion starts to destroy at smaller coupling between planes: $J_1 = 0.015J$ for the ferromagnetic exchange between planes and $J_1 = -0.05J$ for the antiferromagnetic exchange. These results are tempting to think that in real cuprates (where $J_1 \sim 10^{-5}J$) the exchange coupling between CuO_2 planes doesn't destroy skyrmions.

Thus the magnetic properties of the two-dimensional Heisenberg magnetic at low doping were investigated. Using the method, offered by Waldner [5], the program product that permits to observe in

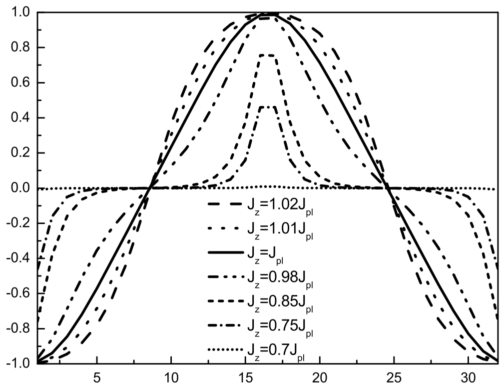

Figure 5: Modification of the skyrmion form in dependence of the exchange coupling anisotropy magnitude. Ferromagnet.

different cases the spin system relaxation to the equilibrium state, was developed. It was shown that the hole introduced into the CuO_2 plane causes the creation of the skyrmion spin configuration by the simulation of the electronic hole behaviour.

The stability of skyrmion state and the influence of the exchange coupling anisotropy and interaction between planes on the form and size of skyrmion was investigated. It was established that at $J_z < J_{x,y}$ the skyrmion tends to turn into the vortex and at $J_z > J_{x,y}$ one can see the tendency to the formation of the domain structure. Also the interaction between planes was investigated. The case of two weak-interacted planes (like in $YBa_2Cu_3O_6$) and completely three-dimensional case (like in La_2CuO_4) were considered. It was shown that the ferro- and antiferromagnetic interaction between planes leads to the destroying of the skyrmion state at the sufficiently large magnitude of the interaction. As a result it was established that in real cuprates the anisotropy of exchange coupling and the interaction between planes are much less than the critical values at which skyrmion spin configuration begins to destroy.

References

[1] Shraimann B.I., Siggia E.D., *Phys. Rev. Lett.*, v. **61**, N.4, 467 (1988)

[2] R.J. Gooding, *Phys. Rev. Lett.*, v. **66**, N.17, 2266 (1997)

[3] T. Morinari, *arXiv: cond-mat*/0502437 (2005)

[4] A.I. Ahiezer, V.G. Bariahtar, S.V. Peletminsky, *JETP*, v. **36**, 474 (1967)

[5] F. Waldner, *Abstracts of international conference on theoretical trends in low-dimensional magnetism.* Firenze, p.32 (2003)