

Destruction of Magnetic Long-Range Order by Hole-Induced Skyrmions in Two-Dimensional Heisenberg Model

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Motivated by the rapid destruction of antiferromagnetic long-range order in hole-doped cuprate high-temperature superconductors, we study the effect of skyrmions on the magnetic long-range order (MLRO). Here we assume that either a skyrmion or antiskyrmion is introduced by a doped hole. Our numerical simulation indicates that in the case of isolated skyrmions, there is an abrupt disappearance of MLRO for doping concentration \( x < 1.0 \times 10^{-4} \). In the case of skyrmion-antiskyrmion pairs, the critical doping concentration \( x_c \) for the suppression of MLRO is given as a function of the separation of the pairs. For a moderate separation of 3 – 4 lattice constants, we find that the critical doping is consistent with the experimental value.

1. Introduction

The parent compounds of the cuprate high-temperature superconductors are Mott insulators.1 Each hole at the copper sites is localized by the charge-transfer gap.2 These localized spin-1/2 moments are well described by the two-dimensional antiferromagnetic (AF) Heisenberg model, and it is now well established that the ground state is the antiferromagnetic long-range-ordered (AFLRO) state.3 High-temperature superconductivity takes place upon hole doping in such parent compounds.

In order to uncover the mechanism of high-temperature superconductivity and the physics underlying the intriguing pseudogap phenomenon4 observed above the superconducting transition temperature, it is necessary to figure out how doped holes are described in the cuprate high-temperature superconductors. In slightly hole doped compounds, the AFLRO state is rapidly destroyed by hole doping.5

Timm and Bennemann6 studied the effect of vortices on the AFLRO state. They considered vortices induced by doped holes as well as thermally excited vortices. The Néel temperature was computed using extended Berezinskii–Kosterlitz–Thouless renormalization group theory and good agreement with the experimentally observed critical doping \( x_c \approx 0.02 \) was obtained.

In this paper, we consider skyrmions instead of vortices. It is natural to consider that vortices destroy magnetic long-range order (MLRO) in the XY model. The field in the XY model is the U(1) phase field. Thus, a topological defect in such a U(1) theory is a vortex. On the other hand, the low-energy effective theory for the AF Heisenberg model is the O(3) nonlinear \( \sigma \)-model.7,8 A topological defect in theories with O(3) symmetry is a skyrmion configuration. If we denote the angle of the XY spin by \( \phi \), a single vortex solution existing at the origin is \( \phi = \tan^{-1}(y/x) \). This vortex is interpreted as a gauge flux with the vector potential

\[
\partial_y \phi = -x/r^2, \quad \partial_x \phi = y/r^2. \tag{1}
\]

This flux is singular at the core of the vortex, and the winding number is one for vortices. Thus, this is a topological defect. In the case of the Heisenberg model skyrmions are exact solutions of the O(3) nonlinear \( \sigma \) model that describes the low-energy effective theory of the AF Heisenberg model.7,8 In the CP\(^1\) representation9 of the nonlinear \( \sigma \) model, such a skyrmion solution turns out to be the gauge flux \( \partial_y a_y - \partial_x a_x \) with

\[
a_x = \frac{y}{r^2 + \lambda^2}, \quad a_y = \frac{x}{r^2 + \lambda^2}. \tag{2}
\]

Here \( \lambda \) is the size of the skyrmion. The skyrmion configuration is a topological defect characterized by the homotopy group \( \pi_2(S^2) \cong \mathbb{Z} \). Note that Eq. (2) coincides with Eq. (1) when taking the limit \( \lambda \to 0 \). In contrast to vortices in the XY model, the singularities at the positions of the vortices are relaxed by a finite parameter \( \lambda \). For these reasons, it is natural to consider skyrmions instead of vortices in the Heisenberg model. However, it has not yet been established how a doped hole creates a skyrmion microscopically. Numerical study of the Hubbard model within the unrestricted Hartree–Fock approximation10 suggests the existence of many nearly degenerate metastable configurations and that a vortexlike spin configuration is formed around the holes. An unrestricted spin-rotational-invariant slave-boson approach12 suggests that a vortex-antivortex pair has lower energy than the Néel-type bipolaron for two holes doped in the half-filled Hubbard model. An effective Hamiltonian approach based on the t-J model13,14 suggests that a long-range dipolar distortion of the staggered magnetization is created around doped holes. Skyrmions have been investigated using the analogies between pions in QCD and magnons in antiferromagnets.15,16 A finite-size-cluster calculation suggests the stability of a skyrmion around a localized doped hole.17–19 Ex-

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experimentally, the existence of skyrmions in AF insulators has been supported by the low-temperature magnetic and transport properties of slightly Li-doped La$_2$CuO$_4$.\textsuperscript{20}

In this paper we numerically simulate the destruction of the AFLRO state assuming that doped holes induce skyrmions. We examine two cases: one is that isolated skyrmions are introduced by doped holes; the other is that skyrmion-antiskyrmion pairs are introduced by doped holes. We find that isolated skyrmions are too strong to destroy the AFLRO state. The same is true for skyrmion-skyrmion pairs. If we consider a skyrmion-antiskyrmion pair with a moderate separation, the critical doping $x_c$ is in good agreement with the experimental value.\textsuperscript{5}

The outline of this paper is as follows. In Sect. 2 we describe the model and the numerical simulation procedure. In Sect. 3 we present the numerical simulation results. Finally Sect. 4 is devoted to a conclusion.

2. Model

In order to investigate the effect of skyrmions on the AFLRO state, we randomly distribute skyrmions or antiskyrmions in the spin system. For comparison, we also investigate the effect of vortices on magnetic long-range order in the XY model. In that case, we randomly distribute vortices or antivortices in the spin system.

Here we focus on the doping concentration at which the system is insulating for the cuprates. Thus, we neglect the effect of itinerant electrons. There is a possibility that the doped-hole wave function is not restricted to a single site but is spread over several lattice sites. Although such a wave function might lead to the stabilization of skyrmions,\textsuperscript{17} we do not include it to simplify the numerical simulation.

For the distribution of skyrmions, we consider two cases. One is a completely random distribution of skyrmions and antiskyrmions with the constraint that the number of skyrmions is equal to the number of antiskyrmions. The other is a random distribution of skyrmion-antiskyrmion pairs. We consider the same distributions for the case of vortices in the XY model.

Since we are interested in the spin system with MLRO, we may consider classical spins. The effect of quantum fluctuations can be included by reducing the size of spins, which leads to renormalization of the exchange interaction $J$ between spins. We take a square lattice with a size of $N \times N$, and the Hamiltonian is given by

$$H = J \sum_{\langle i,j \rangle} S_i \cdot S_j,$$  \hspace{1cm} (3)

where $S_i$ is the localized spin at site $i$ and the summation is taken over the nearest-neighbor sites. In the case of XY spins, $S_i$ is a two-dimensional vector, $S_j = S(\cos \phi_j, \sin \phi_j)$ with $S$ the size of the spin. In the case of Heisenberg spins, $S_j$ is a three-dimensional vector, $S_j = S(\sin \theta_j \cos \phi_j, \sin \theta_j \sin \phi_j, \cos \theta_j)$. For classical spins, one can transform antiferromagnets to ferromagnets on bipartite lattices by reversing the direction of spins at odd sites. Thus, we may consider a ferromagnet instead of an antiferromagnet.

We assume that skyrmions or vortices are induced by doped holes. We denote the number of doped holes by $N_h$. The doped hole concentration is defined by $x = N_h/N^2$. In the case of vortices in the XY model, the randomly distributed $N_h$ vortices are described by

$$\phi_j = \sum_{\ell=1}^{N_h} q_{\ell} \tan^{-1} \left( \frac{y_j - y_{\ell}}{x_j - x_{\ell}} \right),$$  \hspace{1cm} (4)

where $x_j$ and $y_j$ denote the coordinate of lattice site $j$ and $q_{\ell} = 1$ for vortices and $q_{\ell} = -1$ for antivortices. The vortex positions are denoted by $(x_{\ell}, y_{\ell})$, and random integer numbers ranging from 1 to $N$ plus one-half are assigned to $x_{\ell}$ and $y_{\ell}$. Thus, vortices are introduced at the centers of plaquettes.

In the case of skyrmions in the Heisenberg model, we make use of the form of Eq. (4). We fix the size of the skyrmion $\lambda$ to the lattice constant.\textsuperscript{17} We determine the polar angle $\theta_j$ of the Heisenberg spin, which is absent in the XY spin, through the minimization of the energy of the spin system. We realign each spin so that it is in the direction of the local average of the four surrounding spins. We update the spin configuration while keeping the directions of the four spins surrounding the skyrmion or antiskyrmion fixed. This is necessary to maintain the skyrmion configurations because skyrmions are metastable in the Heisenberg model. In order to stabilize skyrmions, we require additional interactions, such as the Dzyaloshinskii–Moriya interaction or frustrated interaction. However, the mechanism by which skyrmions in the cuprates are stabilized has not been established yet, and so we simply introduce the fixing procedure above to maintain the skyrmions. We carry out the update procedure until the self-consistent spin configuration is obtained.

3. Numerical Simulation of MLRO Destruction

In order to measure the effect of MLRO destruction by skyrmions, we analyze the skyrmion concentration dependence of the magnetization, $M(N) = \sqrt{\sum_{i=1}^{N^2} S_i^z}/(N^2 S)$, which is normalized by the maximum magnetization, $N^2 S$. The thermodynamic limit of the magnetization, $M_0 = \lim_{N \rightarrow \infty} M(N)$, is obtained from finite-size scaling assuming that $M(N) = M_0 + M_1/N^2 + M_2/N^4 + \cdots$. We carried out the numerical simulation for $N = 128, 256, 512$.

A simple random configuration is obtained by distributing skyrmions and antiskyrmions completely randomly by choosing $N_h$ sites out of $N^2$ sites. However, this completely random configuration leads to the abrupt disappearance of MLRO. The critical value of $x$ is less than $10^{-4}$. The situation is almost the same for the case of vortices in the XY model. Note that here we set $\lambda$ equal to the lattice constant. This choice corresponds to the half-skyrmion.\textsuperscript{21,22} In the CuO$_2$ plane there is a strong correlation of stabilizing the Zhang–Rice singlet.\textsuperscript{23} If a doped hole forms the Zhang–Rice singlet with a copper site spin, then the spin is removed at the doped hole position. The singlet state tends to stabilize a half-skyrmion-like spin configuration as discussed in Ref. 17. For larger values of $\lambda$, the
disorder introduced by skyrmions becomes stronger. Meanwhile, the case of \( \lambda = 0 \) must be considered separately. In this case, only local spin flips are introduced, and the magnetization immediately recovers the bulk value away from holes. Thus, we simply obtain \( M = 1 - 2x \), which is inconsistent with the rapid destruction of MLRO in the cuprates.

A completely random configuration ignores the interaction effect between skyrmions as well as the Coulomb interaction between holes. If we denote the separation of a skyrmion-antiskyrmion pair by \( d \), the energy of a single pair depends on \( d \). Figure 1 shows the energy \( E_d \) of a skyrmion-antiskyrmion pair as a function of \( d \). We computed the energy of a single pair whose direction is either horizontal or diagonal. For \( d > 3 \), the energy does not depend on the direction of the pair. The energy saturates for large \( d \), which can be interpreted as meaning that the pair is almost decoupled and the configuration of pairs cannot be distinguished from completely randomly distributed skyrmions. Meanwhile, for \( d < 3 \), the result slightly depends on the direction of the pair. The effect of the Coulomb energy \( E_C \) between doped holes is shown in the inset of Fig. 1. Note that \( E_d + E_C \) is a monotonically decreasing function with respect to \( d \). On the other hand, the average distance between the doped holes is given by \( 1/\sqrt{d} \) in units of the lattice constant. For the case of \( x = 0.02 \), we find that \( 1/\sqrt{d} \approx 7.1 \). The value of \( 1/\sqrt{d} \) gives an upper bound for \( d \). Thus, we may consider \( 1 < d < 7 \) when examining the effect of skyrmion-antiskyrmion pairs on MRLO.

We carried out numerical simulations for different values of \( d \). In units of the lattice constant, we take \( d = 1, 2, 3, 4, 5, 6 \) for pairs aligned horizontally and \( d = \sqrt{2}, 2 \sqrt{2}, 3 \sqrt{2}, 4 \sqrt{2}, 5 \sqrt{2} \) for pairs aligned diagonally. The configurations of the pairs are determined randomly. In order to ensure that the separation of the pairs is the prescribed value \( d \), we first choose \( N_s/2 \) consecutive sites of size \( d + 1 \) without overlapping and then place skyrmion-antiskyrmion pairs at both their ends.

The number of samplings is 20, which appears to be sufficient as we did not observe significant improvement of the convergence by increasing the number of samplings. We found systematic variation of the \( x \)-dependence of the magnetization upon increasing \( d \) as shown in Fig. 2. For \( d \leq 3 \), which is in the parameter range where the single pair energy depends on the pair direction, \( M \) decreases slowly and almost linearly with respect to \( x \).

This gradual destruction of MLRO by skyrmion-antiskyrmion pairs changes to rapid destruction for \( d \geq 4 \) as shown by the convex downward curves.

The difference between these two cases is clarified when we see the spin configuration and topological charge distribution. The topological charge density on the lattice is defined by

\[
q(x_j,y_j) = \frac{1}{16\pi} \left[ n(x_j, y_j) \cdot n(x_j + 1, y_j) \times n(x_j + 1, y_j + 1) \right. \\
+ \left. n(x_j - 1, y_j) \times n(x_j, y_j - 1) \right] \\
+ \left. n(x_j, y_j + 1) \times n(x_j - 1, y_j) \right] \\
+ n(x_j, y_j - 1) \times [n(x_j + 1, y_j)] ,
\]

where \( n(x_j, y_j) = S_j / S \). Figure 3 shows the spin configuration for the case of \( d = 2 \). In spite of the fact that we introduced skyrmions, almost all the spins lie in the \( x-y \) plane. Reflecting this feature, there is almost no topological charge density distribution over the system. In contrast, in the case of \( d = 6 \), both the spin configuration and the topological charge density distribution shown in Fig. 4 suggest that there is a significant
effect of skyrmion-antiskyrmion pairs on the spin configuration. Although the topological charge density is not directly connected with the disorder of spins, as one can see from Fig. 4, the rapid change in the sign of the topological charge density over the sites implies the presence of strong disorder.

Now we discuss the critical doping concentration. We stop the update procedure when the maximum difference between the spin values after the update and those before the update is less than $10^{-6}$. Thus, for the size of $512 \times 512$, the value of $M \sim 0.1$ corresponds to the complete destruction of MLRO. Therefore, we may conclude that MLRO should disappear around $0.02 < x < 0.04$ for $d > 3$. From the discussion above, the Coulomb repulsion increases $d$, the separation of skyrmion-antiskyrmion pairs, while there is an upper limit of $1/\sqrt{x}$ for $d$. Thus, the rapid destruction of MLRO by skyrmion-antiskyrmion pairs is consistent with that observed in the cuprates.

For comparison, we carried out similar numerical simulations for the case of vortex-antivortex pairs introduced in the XY model. The result is shown in Fig. 5. Interestingly, we obtained a similar result.

In order to find the critical value of $d$, we computed the energy of the system. Figure 6 shows the $d$ dependence of the system energy for $x = 0.02$, which consists of the energy of the spins and the Coulomb interaction energy between the holes. The system energy shows a minimum around $d \sim 4$. The appearance of this minimum is a natural consequence of the competition between the energy of the spins and the Coulomb interaction energy between the holes. Basically, the energy of the spins increases monotonically with increasing $d$. Meanwhile, the Coulomb interaction energy decreases monotonically with increasing $d$. This is understood from an approximate calculation. An approximate formula for
the Coulomb energy is given by

$$E_C(d) = \frac{e^2}{4\pi\varepsilon} \left( \frac{N^2 x}{2d} + \frac{3}{2} N^3 \varepsilon^2 \right).$$

(6)

This formula is obtained by finding an approximate formula for the Coulomb energy of two skyrmion-antiskyrmion pairs, and then computing the total energy of randomly distributed skyrmion-antiskyrmion pairs. The term proportional to $N^3$ on the right-hand side of Eq. (6) is the dominant term. For the case of $x = 0.02$ and $N = 256$, we find that its value is 2250 K per site. This is consistent with Fig. 6. However, this value is $d$-independent. We confirmed that the energy takes a minimum around $d \sim 4$ for different values of $x$ ranging from 0.01 to 0.05. The critical value of $d$ depends on $\eta = e^2 / (4\pi\varepsilon a JS^2)$ with $a$ the lattice constant. For the cuprates, $\eta = 44.4$ with $\varepsilon = 3\varepsilon_0$ and $S = 1/2$. However, the critical value of $d$ does not change much upon changing $\eta$ from 30 to 120. Thus, even if there is a reduction of the size of the spin due to the quantum fluctuations, the critical value of $d$ is the same. Note that the statistical error for the energy calculation is significant. Thus, we were unable to evaluate the binding energy of the skyrmion-antiskyrmion pair.

4. Conclusions

We have examined the effect of skyrmions on MLRO in the Heisenberg model. We have assumed that the size of the skyrmion, $\lambda$, is equal to the lattice constant. Either a skyrmion or antiskyrmion is introduced by doping holes in the system. We found that the effect of isolated skyrmions and antiskyrmions is too strong to destroy MLRO. For the case of skyrmion-antiskyrmion pairs, which are expected to be formed because of the Coulomb repulsion between holes and the interaction between skyrmions, we found that the critical hole doping concentration is consistent with the experimental values for the cuprates. Since the appropriate pair separation is almost equal to the average hole distance $1 / \sqrt{\lambda}$, our numerical simulations suggest that doped holes are almost uniformly distributed and that there is an antiferromagnetic configuration of skyrmions and antiskyrmions.

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