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The interaction of a magnetic vortex with the frustration created by a magnetic defect is investigated in a discrete Heisenberg model of a two-dimensional antiferromagnet with easy-plane anisotropic exchange. Numerical solutions are obtained for the static Landau-Lifshitz equations describing the spin distribution in a system with magnetic frustration and a vortex. It is found that the energy of the magnet is minimum in the case when the center of the vortex coincides with the position of the magnetic impurity. It is shown that as a result of the attraction between the vortex and frustration, a two-dimensional solitonic bound state localized at the magnetic defect—a frustrated vortex—arises in the magnet. The energy of such a vortex is lower than that of the free vortex, and this effect can be manifested in features of the behavior of the EPR linewidth in two-dimensional magnets. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2008133]

I. INTRODUCTION

The class of quasi-two-dimensional antiferromagnets comprising metalorganic compounds can evidently be supplemented by high-T_c superconductors in the magnetically ordered phase.[1] The CuO_2 planes in high-T_c superconducting compounds such as $YBa_2Cu_3O_{6+x}$ and $La_{2-x}Sr_xCuO_{4-y}$ are two-dimensional Heisenberg layers of antiferromagnetically coupled copper spins with a value close to 1/2.[2] The superexchange J between Cu^{2+} ions takes place through the oxygen ions O^{2-}. These almost isotropic two-dimensional layers are coupled by a weak exchange $J_\perp \ll J$ of the same order as the easy-plane magnetic anisotropy.[3] It is known[4] that the electronic state of the CuO_2 planes and, hence, the character of the magnetic exchange between Cu^{2+} ions depend substantially on the oxygen content in high-T_c superconductors. In particular, it has been established for lanthanum and yttrium superconductors that variation of the oxygen concentration leads to the formation of "holes" in the CuO_2 plane. These "holes" are charge carriers in the superconducting phase,[5] and in the opinion of Aharony and co-authors,[2] their localization at the oxygen in the magnetic phase leads to a change in character of the superexchange between the Cu^{2+} ions, from antiferromagnetic with $J \approx 1000$ K to ferromagnetic with $J' \approx -3000$ K.[3] The resulting frustration[6] destroys the long-range magnetic order.

The quantum description of these phenomena is a very laborious task,[7] and for that reason the analytical approach usually turns to the framework of classical Heisenberg models.[8] In the Heisenberg XYZ model the magnetic interactions in the copper planes in $YBa_2Cu_3O_{6+x}$ are described by a Hamiltonian of the form

$$H_0 = J\sum_{\mathbf{r},\mathbf{a}} [S^x_{\mathbf{r}} S^x_{\mathbf{r}+\mathbf{a}} + \eta S^y_{\mathbf{r}} S^y_{\mathbf{r}+\mathbf{a}} + \lambda S^z_{\mathbf{r}} S^z_{\mathbf{r}+\mathbf{a}}], \tag{1}$$

on a square lattice, where $\mathbf{S_r}$ is the classical spin, the summation is over lattice sites and nearest neighbors, the constant $\lambda < 1$ corresponds to easy-plane anisotropy, and the constant η is introduced to take into account a weak anisotropy in the plane: $1-\eta \ll 1-\lambda \ll 1$. It will be understood that the results obtained below are applicable primarily to yttrium compounds, for which $\lambda \approx 0.99$, whereas for lanthanum compounds it is important to take the Dzyaloshinski–Moriya interaction into account as well. For yttrium compounds, since the spins of two nearest-neighbor copper planes interact antiferromagnetically with an exchange $J_\perp$, we shall assume when studying the static configurations that the nearest spins in different planes are pairwise antiparallel.

The static spin distributions are solutions of the following Landau-Lifshitz equations:

$$\mathbf{S_r} \times \mathbf{F_r} = 0, \quad \mathbf{F_r} = -\frac{\delta H}{\delta \mathbf{S_r}}, \tag{2}$$

where $\mathbf{F_r}$ is the effective field at site $\mathbf{r}$, and H is the Hamiltonian of the magnetic system. In the presence of a bond defect (the exchange constant between two spins has a different sign from the interaction in the host matrix), as a result of frustration, the ground state can be nonuniform (in the XY model this is a threshold effect in the parameter J'/J).[7] Such a state, with a nonuniform distribution of the antiferromagnetic vector field localized near the defect is called a Villain ground state.[6] On the other hand, such a localized spin structure can also be interpreted naturally as a two-dimensional magnetic soliton localized at the defect. Therefore, the term magnetic frustration has come to denote a solitonic spin distribution arising near an effective frustrated bond.[2] Such frustrations can influence the magnetic characteristics of high-T_c superconducting (HTSC) compounds, in particular, the temperature of the Néel phase transition in $YBa_2Cu_3O_{6+x}$ (Ref. 9), and can contribute to the susceptibility of the crystals. Direct experimental measurement of the susceptibility of the CuO_2 planes is difficult because of the large values of the exchange constants J and J'. However, it has become possible to estimate the susceptibility of the

CuO_2 layers in an indirect way thanks to the discovery of a new class of HTSC compounds containing rare-earth (R) ions: $GaBa_2Cu_3O_{6+x}$, $Nd_{2-x}Ce_xCuO_4$, etc.,[10,11] in which the rare-earth ions neighbor the CuO_2 planes. A soliton approach to the treatment of questions related to the structure of magnetic frustrations in the CuO_2 layers of HTSC compounds and their rare-earth analogs in the presence of magnetic field was proposed in Refs. 12 and 13; the contribution of frustrations to the magnetic susceptibility of magnets was investigated, and the magnetic fields induced by the field of a frustration in the rare-earth ion layers were found. Since the characteristic interactions in the rare-earth layers are substantially smaller than the exchange J in the CuO_2 plane, the magnetic properties of the planes containing the Ga, Nd, etc. ions are studied by conventional techniques. Susceptibility measurements in compounds of the class R_2CuO_4 have revealed[11] weak ferromagnetism, one of the causes of which may be that frustrations having a magnetic moment are present in the CuO_2 planes. Since frustrations in the CuO_2 planes influence the magnetic ordering in the adjacent rare-earth layers,[13] one expects that frustration contributions will also be manifested in magnetic resonance experiments.

On the other hand, it is well known that magnetic vortex solitons can exist in two-dimensional isotropic and easy-plane magnets.[14,15] In the case of weak anisotropy these vortices have a structure with spin components that come out of the plane.[16] Such solitons can contribute to the EPR line broadening in quasi-two-dimensional magnets.[17,18] Their interaction with magnetic and nonmagnetic defects of substitution has become a topic of research only recently.[19–23]

In this paper we investigate the character of the interaction of a magnetic frustration and a vortex in an easy-plane antiferromagnet and predict the formation of their bound state—a *frustrated vortex*. Such nonlinear excitations can contribute to the resonance and thermodynamic characteristics of quasi-two-dimensional magnets and HTSC compounds in the magnetically ordered phase.

II. TWO-DIMENSIONAL HEISENBERG MAGNET WITH A FRUSTRATING IMPURITY

The use of a planar model for describing magnetic frustration,[2,8,12] raises the question of the correctness of replacing the almost isotropic Heisenberg Hamiltonian customarily used for HTSC compounds by the XY model. The important circumstance that calls the applicability of such an approximation into question is this: two-dimensional solitons—magnetic vortices—can exist in easy-plane magnets.[14,16] If the anisotropy is not small, then the vortex spin configuration is planar. In the almost isotropic case, which corresponds to the CuO_2 plane, the vortex configuration acquires spin components that come out of the plane. This naturally raises the questions of how the magnetic frustrations will behave in an almost isotropic Heisenberg model, and what will be the nature of the interaction of a frustration and a magnetic vortex in such a system?

To answer these questions, we formulate the following classical model describing the interaction of the spin of a hole and the spins of the copper in the CuO_2 plane (see also Ref. 7). The Hamiltonian (1) is supplemented with a term appropriate to such an interaction:

$$H=H_0+H_{\mathrm{fr}},\quad H_{\mathrm{fr}}=\tilde{J}\mathbf{S}_h\cdot(\mathbf{S}_{\mathbf{r}_1}+\mathbf{S}_{\mathbf{r}_2}),\tag{3}$$

where $\mathbf{S}_h$ is a hole spin, and the exchange $\tilde{J}$ between the hole spin and a copper spin is assumed, for the sake of definiteness, to be antiferromagnetic, i.e., $\tilde{J}>0$. (We recall that all of the spins have been replaced by classical unit vectors, and their absolute value $S=1/2$ is subsumed in the renormalization of the exchange constants.) This model explicitly takes into account the interaction of the magnetic impurity with the spins of the host and admits a transition in terms of this parameter to the defectless case, $\tilde{J}\to 0$. We note that the static Landau-Lifshits equation for the hole spin,

$$\mathbf{S}_h\times(\mathbf{S}_{\mathbf{r}_1}+\mathbf{S}_{\mathbf{r}_2})=0\tag{4}$$

has the obvious solution in accordance with the fact that the hole spin is antiparallel to the sum of the copper spin vectors:

$$\mathbf{S}_h=-\frac{\mathbf{S}_{\mathbf{r}_1}+\mathbf{S}_{\mathbf{r}_2}}{|\mathbf{S}_{\mathbf{r}_1}+\mathbf{S}_{\mathbf{r}_2}|}.\tag{5}$$

Therefore, in the proposed model the frustrated contribution of the hole to the interaction between the statically distributed copper spins is equal to $H_{\mathrm{fr}}=-\tilde{J}|\mathbf{S}_{\mathbf{r}_1}+\mathbf{S}_{\mathbf{r}_2}|$. We note that the effective interaction of the copper spins via the hole spins turns out to be of a ferromagnetic character independently of the initial sign of the interaction of the hole spin and copper spin (see also Ref. 2). Here we note that, unlike the models using the frustrated bond approximation,[2,8] which lead to results that are equivalent for ferro- and antiferromagnets to within a change of the signs of the exchange constants, the present model pertains specifically to antiferromagnets, since it is due to the inevitable frustrating influence of an interstitial magnetic impurity on the antiferromagnetic ordering of the host spins.

The solution (5) of equation (4) suggests a numerical algorithm that permits effective solution of the static equation (2) in the general case. An iterative method of solving the static Landau–Lifshitz equations for arbitrary values of the spins S and arbitrary interactions governing the equilibrium state of the system (in particular, spin distributions like two-dimensional magnetic frustrations and vortices) is based upon the following idea. It follows from Eq. (2) that the vector $\mathbf{S}_{\mathbf{r}}$ should always be parallel to the effective field $\mathbf{F}_{\mathbf{r}}$, and the elementary iteration step can therefore be written as

$$\mathbf{S}_{\mathbf{r}}^{i+1}=S\cdot\mathbf{F}_{\mathbf{r}}^{i}/F_{\mathbf{r}}^{i},\tag{7}$$

where $F_{\mathbf{r}}^i$ is the length of the vector $\mathbf{F}_{\mathbf{r}}^i$, and the index i is the number of the iteration. If the initial spin distribution if sufficiently close in form to a magnetic frustration or vortex, then the iterative calculation converges very rapidly and leads to a stable solution of Eqs. (2).

III. INTERACTION OF A MAGNETIC FRUSTRATION AND A VORTEX IN A TWO-DIMENSIONAL ANTIFERROMAGNET

In this paper we report a numerical investigation of the equilibrium spin configurations in the framework of the discrete Heisenberg model (3) on a 41×40 spin matrix (n,m) (the lattice constant is taken equal to unity). First we obtained solutions describing magnetic frustrations; they turned

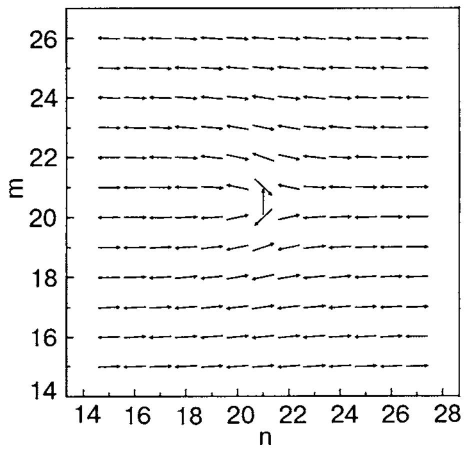

FIG. 1. A 13×12 fragment of the spin distribution at a magnetic frustration. The positions of the central spins are the sites (21,20) and (21,21), between which is located the spin of a magnetic impurity.

out to be practically the same as in the planar model,[2,8,12,13] i.e., localized in the easy plane at for arbitrarily weak anisotropy (see Fig. 1). This circumstance permits a complete justification of the use of the planar model for calculating the structure of the frustrations in the presence of magnetic field.[12,13] We note that in the purely isotropic case ($\eta=\lambda=1$), all the spins of the frustration also lie in a single plane, but there is degeneracy with respect to rotation of that plane around an arbitrary axis. In the frustration model with interaction (3) a nonuniform ground state arises at arbitrarily small values of the parameter $W=\tilde{J}/J$. For $W=0$ the energy of the uniform antiferromagnetic ground state of a 41×40 matrix of spins in units of J has the value $E_0=-3199$. The energy of the system with frustration, E_{fr}, initially falls off quadratically as a function of the parameter W but then, after $W\approx 3$, its decline becomes practically linear (Fig. 2). Thus the energy of the system with frustration is lowered by an amount $\Delta E_{\text{fr}}=E_{\text{fr}}-E_0$, which is naturally called the self-energy of a frustration. For example, for $W=3$ the energy $\Delta E_{\text{fr}}=-2.08$.

The proposed numerical method is efficient for calculating the structure of a vortex with components that come out from the easy plane, since in that case the spin distributions in the course of the iterations converge rapidly to the stable solutions. As the initial distribution for the vortex in the calculations we used approximate analytical expressions for easy-plane vortices from Ref. 16. The numerical calculation

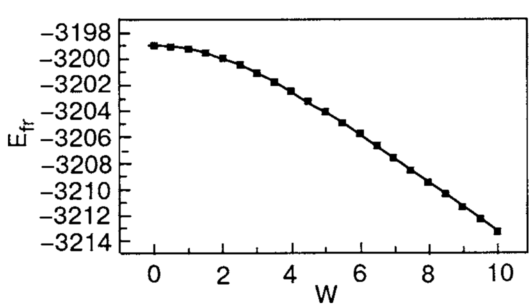

FIG. 2. Energy of an antiferromagnet with frustration E_{fr}, measured in units of J, as a function of the frustration interaction parameter W.

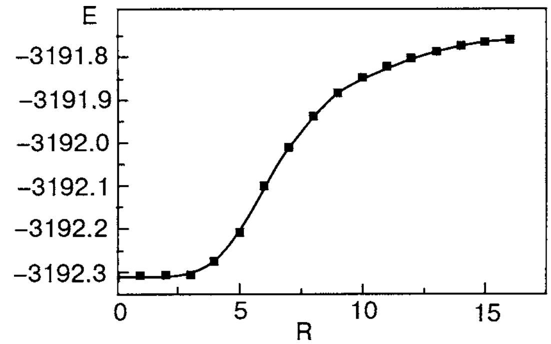

FIG. 3. Energy of an antiferromagnet containing a vortex and a frustration, measured in units of J, as a function of the distance between their centers.

for the energy of a free vortex (i.e., in the system without a frustrating impurity, $W=0$) for a 41×40 spin matrix gives $\Delta E_v=E_v-E_0=9.51$.

The next step consists in the calculation of the interaction of a magnetic vortex and a frustration in the framework of the proposed model. For this the problem is stated for the following physical situation: a hole is introduced into a system of spins with a vortex at the center and is moved to different distances from the center of the vortex. It was assumed in the calculations that the anisotropy constants $\eta=1$ and $\lambda=0.99$, and the ratio of exchange constants $W=3$. For the stable configuration obtained, the energy of the system was found. Figure 3 shows the dependence of that energy on the distance R between the hole spin and vortex center. It is seen that the interaction is of an attractive character. It follows from an analysis of the spin distributions obtained that at large distances between the hole spin and vortex center the presence of frustration is practically unnoticeable (see Fig. 4), and outwardly the vortex differs little from the free vortex.[16] At the same time, the vortex turns out to be strongly deformed in the energetically most favorable state, when the vortex center lies on the axis between two copper spins, coinciding precisely with the position of the hole spin (Fig. 5). Such a bound state of the magnetic vortex and an impurity spin is naturally called a *frustrated vortex*. The strong frustrating influence of the magnetic impurity on the deviation of the components of the vortex from the easy plane is clearly seen in Fig. 6, which shows the modulus of the $S^z_{\mathbf{r}}$ components of the host spins.

To find the energy ΔE_{fv} of a frustrated vortex, one must subtract from the total energy $E_{fv}=-3192.31$ the energy

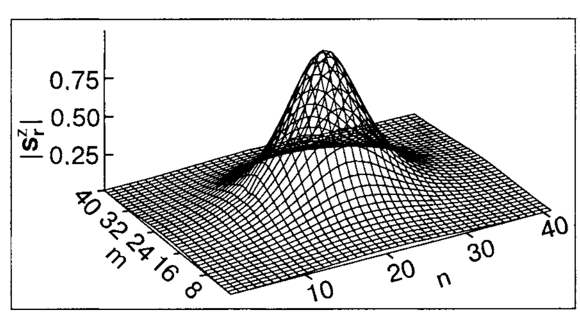

FIG. 4. Modulus of the projection $S^z_{\mathbf{r}}$ on the coordinates in an antiferromagnet containing a vortex and a magnetic frustration in the case when the impurity spin is located between sites (11,20) and (11,21).

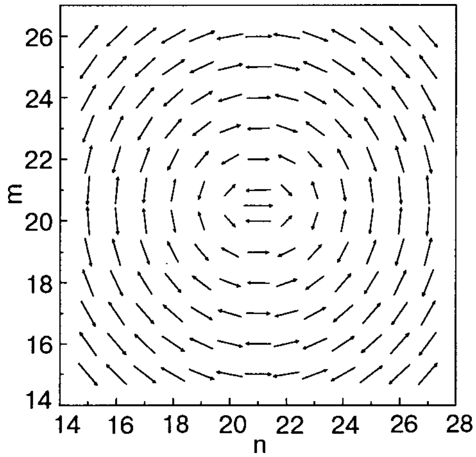

FIG. 5. A 13×12 fragment of the distribution of the projections of spins in a frustrated vortex. The arrows indicate the components of the vectors $\mathbf{S}_\mathbf{r}$ in the XY plane. The impurity spin is located in the middle between sites (21,20) and (21,21).

$E_{\mathrm{fr}} = -3201.08$ of a nonuniform ground state of the system with an isolated frustration. The energy obtained, $\Delta E_{fv} = 8.77$, is less than the energy ΔE_v of a free vortex by the amount of the binding energy, $\Delta E_b = -0.74$, which amounts to around 8% of the vortex energy. As is seen in Fig. 3, these calculations are equivalent to finding the binding energy in a frustrated vortex by subtracting from E_{fv} (the total energy at $R=0$) the energy of the system with the magnetic frustration removed to a large distance and the free vortex.

Returning to the initial physical statement of the problem, we emphasize that introducing a hole into a CuO_2 plane containing a free vortex leads to the formation of their bound state—a frustrated vortex, and lowers the energy of the system as a whole by an amount $\Delta E = -2.82$, which consists of the energy of a frustration and the binding energy.

Thus, for given dimensions of the lattice (or density of vortices and holes) and values of the exchange interactions, a numerical estimate of the energy of a frustrated vortex shows that the decrease of the system energy due to the introduction of a hole into it and the localization of the vortex at the hole is of the order of 30% of the energy of a free vortex.

Such a decrease might be detected in EPR experiments in layered magnets—rare-earth analogs of HTSC compounds. Upon localization of the magnetic impurity at a site in a metalorganic antiferromagnet one observes temperature broadening of the EPR line. One of the possible explanations for this is that this broadening of the resonance line includes a contribution from magnetic vortices.[17] An estimate of the energy of the vortices can be obtained from the temperature dependence of the EPR linewidth.[18] In HTSC compounds EPR directly on the copper ions is not observed; this remains one of the unexplained mysteries of the physics of high-temperature superconductivity.[24,25] This may be because of the very strong broadening of the resonance line in these compounds, which may include a contribution from magnetic vortices. The resonance *is* observed in the rare-earth analogs of HTSC compounds,[11] and the contribution of frustrated vortices might be observed indirectly through the fields induced in the planes of the rare-earth ions, as in the simpler case of a replica of a magnetic frustration.[13] It should be noted, however, that for further generalization of the results to the lanthanum compounds $La_{2-x}Sr_xCuO_{4-y}$ it is necessary to take the Dzyaloshinski–Moriya interaction into account in a consistent way, and also the possible motion of the holes, which requires consideration of more-complex spin Hamiltonians.[26,27]

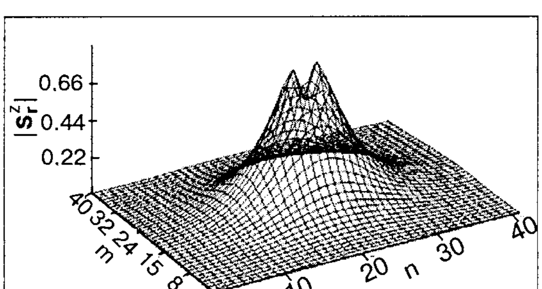

FIG. 6. Frustrated vortex with center of localization at a magnetic defect. The dependence of the modulus of the projection $S_\mathbf{r}^z$ on the coordinates is shown.

IV. CONCLUSIONS

We have formulated a discrete classical Heisenberg model of a two-dimensional antiferromagnet with easy-plane anisotropy of the exchange with an interstitial magnetic impurity. Such a model can describe the behavior of magnetic copper layers of the HTSC compound $YBa_2Cu_3O_{6+x}$ with holes in the CuO_2 planes. We have investigated the interaction of a magnetic frustration and a magnetic vortex in the framework of this model and obtained the following results.

1. We have proposed an efficient algorithm for numerical solution of the static Landau–Lifshitz equations for calculation of the equilibrium stable spin configurations of magnetic systems with an arbitrary character of the spin interactions.

2. The solutions of the Landau–Lifshitz equations corresponding to magnetic frustration and a magnetic vortex with spin components coming out of the easy plane have been found numerically, and the energy characteristics of these solutions have been calculated as functions of the model parameters.

3. We have shown that the energy of a magnet containing a vortex and frustration is minimum in the case when the center of the vortex coincides with the position of the hole. As a result of the attraction between the vortex and frustration a two-dimensional bound state localized at the magnetic defect—a *frustrated vortex*—appears. The energy of such a vortex is lower than that of the free vortex.

4. This effect can be detected in EPR experiments, since an estimate of the energy of magnetic vortices can be obtained from the temperature dependence of the resonance linewidth, to which these nonlinear excitations give an exponential contribution.

Thus in two-dimensional antiferromagnetic systems with interstitial impurities (such as holes in HTSC compounds) the magnetic frustrations and vortices can form bound states having a substantial influence on the thermodynamics and resonance properties of these systems.

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