Localized spin flop transition in a ladder structure with nonmagnetic impurities

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A classical two-leg spin ladder with an antiferromagnetic exchange interaction and easy axis anisotropy in an external magnetic field exhibits a spin flop transition. A single nonmagnetic impurity introduced into this system allows for the formation of a metastable localized spin flop state at a field above the bulk spin flop field. This state will be symmetrically pinned to the impurity. Two neighboring impurities on the same leg will also result in the stabilization of a localized state pinned to the impurities, but in this case the state is not centered on the impurities. [DOI: 10.1063/1.1356034]

The antiferromagnet below the Neel temperature has different susceptibilities which depend on the direction of the applied magnetic field relative to the sublattice magnetization direction. An interesting consequence of this is the spin flop transition. This occurs when a magnetic field is initially along the sublattice magnetization direction and owing to the nature of antiferromagnetic order there will be no net magnetic moment; however, as the field strength is increased there will be a transition to a state where the spins become perpendicular to the field. This is because of the difference between the parallel and perpendicular susceptibilities which in turn affect the energy such that the total energy of the antiferromagnet can be lowered by spin canting in the external field. In a homogeneous system this transition occurs throughout the spin system and it is referred to as a bulk spin flop transition, and the critical field associated with the bulk spin flop transition depends on the magnitudes of both the exchange interaction and anisotropy.

Since the development of multilayers it has been possible to experimentally study the spin flop transition as well as surface effects. In particular, in semi-infinite systems it has been found that there is a localized surface spin flop transition[1,2] that occurs at a lower field than the critical field for the bulk system and recent theoretical work[3–6] has investigated the nature of this localized state. In principle it should also be possible to observe the surface spin flop transition in quasi-one-dimensional magnetic compounds composed of chain-like systems where the ''surface'' corresponds to the chain end. In these compounds chain ends can easily be introduced through nonmagnetic impurities in the compound which result in finite chains of different sizes. If nonmagnetic impurities are put into higher-dimensional lattices their effect is less clear. In this case there will be no definite ''surfaces,'' but the exchange bonds around the impurity will be eliminated or modified and the existence of a localized spin flop state is an open question.

In this work we consider the system between the chain structure and the two-dimensional lattice, namely the two-leg ladder[7] structure. For this particular structure the introduction of one nonmagnetic impurity will not produce a chain end, however, it can significantly modify the effective exchange field around the impurity. The impurity effect is studied here by numerical minimization of the energy of a ladder structure antiferromagnet to obtain the zero temperature spin structure. As for the case of the surface spin flop state, two structures are noticed: There is a localized structure pinned to the impurity which appears when the magnetic field is below the bulk spin flop magnetic field. For higher values of the field the expected bulk spin flop transition is observed. There are also interesting differences in the symmetry of the localized state resulting from a single or a double impurity (two neighboring impurities on a ladder edge). Namely, the single impurity ladder has a symmetric localized spin structure centered on the impurity, whereas the double impurity is at the edge of the localized structure. It is also remarked that the localized structure is metastable and it will persist well below the critical field required for its formation.

This analysis is done for a classical spin system in order to simplify the numerical calculations; however, there are also manganese halide compounds[8] that are quasi-one-dimensional and two-dimensional antiferromagnets. Furthermore, these Mn(II) compounds have a spin of 5/2 so they are also nearly classical and they might be potential systems to use for experimental tests of these results.

The basic ladder structure that is used here has the same isotropic exchange interaction everywhere within the ladder structure as well as easy-axis anisotropy. For this case the uniform structure without impurities has the energy

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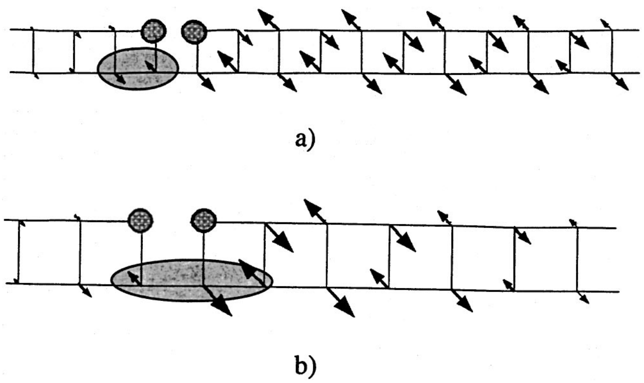

FIG. 1. Ladder structure with two nonmagnetic impurities. For part (a) the magnetic field is $0.96H_{sf}$ and for part (b) the magnetic field is $0.89H_{sf}$. The spins in the shaded ellipse have their z components parallel to the field.

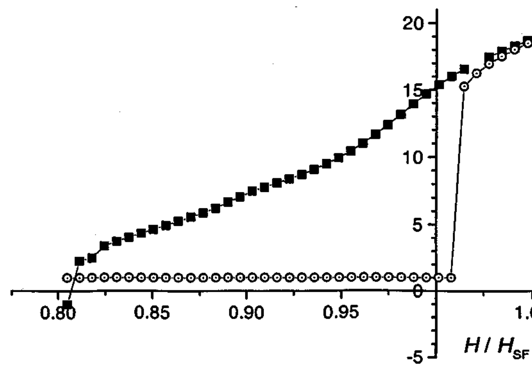

FIG. 3. Total z component of the spin vs magnetic field for the ladder structure with one nonmagnetic impurity. Circles indicate increasing magnetic field and squares indicate decreasing magnetic field.

$$E=J\sum_{i\neq j}\mathbf{S}_i\cdot\mathbf{S}_j-A\sum_{i}(S_i^z)^2-g\mu_B H\sum_{z}S_i^z, \tag{1}$$

where J, A, and H are the exchange and anisotropy constants, and the magnetic field, respectively. In the following, all of the parameters are positive and the length of the classical spin vector is taken to be one; also the first sum is over nearest neighbors with the exchange bonds as well as the two nonmagnetic impurities illustrated in Fig. 1, where the z direction is defined by the magnetic field perpendicular to the ladder plane, and the ladder is in the x direction. As expected this model exhibits a bulk spin flop transition which was found by minimization of the energy for increasingly longer ladders without impurities. This process with $K=0.2J$ gives a spin flop transition at the critical field of $H_{sf}=1.528J/g\mu_B$.

The two different spin structures shown in Fig. 1 were obtained by minimization of the energy for both increasing and decreasing values of the magnetic field. The total z component of the magnetization as a function of the magnetic field is plotted in Fig. 2 with the open circles indicating the increasing field data and the solid squares representing the decreasing field data. Notice that there are two separate hysteresis on this figure. The one that appears at lower values of the field ($0.945H_{sf}$) originates from the formation of the localized state pinned to the two impurities and its structure is

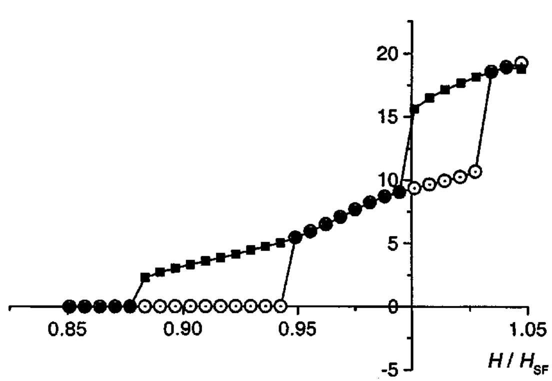

FIG. 2. Total z component of the spin vs magnetic field for the ladder structure with two nonmagnetic impurities. Circles indicate increasing magnetic field and squares indicate decreasing magnetic field.

shown in Fig. 1(a). Here there is Neel-type order throughout the ladder except in the shaded ellipse where the z components of the spins have the same direction, however, the localized nonuniform nature of this state results in the jump in the magnetization shown in Fig. 2. As the field is increased there is another jump at about $1.03H_{sf}$ which is the transition to the bulk spin flop state. Following the solid squares as the field is decreased it is noticed that the bulk spin flop state is metastable down to H_{sf} where there appears a transition again to the localized state. As the field is further decreased the localized state becomes metastable down to about $0.87H_{sf}$ The structure in this second metastable region is shown if Fig. 1(b) where it is noticed that the size of the localized region is smaller, but more interesting is the structure in the immediate vicinity of the impurities. Here the region that does not have Neel-type order in the shaded area has increased to three spins.

For the case of only one impurity the situation is simpler and this case can be used to understand the asymmetry seen in Fig. 1. For one impurity the z component of the magnetization versus the magnetic field is again seen in Fig. 3. In this case, however, there is only one hysteresis with the spin flop state appearing at about H_{sf} as the field is increased. Now as the field is decreased below H_{sf} there is also a localized metastable state that appears which is similar to the state shown in Fig. 1, but it is symmetric about the impurity. Furthermore, this localized state only appears if a spin parallel to the applied field is replaced by the nonmagnetic impurity. This can be understood by considering the energy of the ladder structure with a single impurity. When a spin parallel to the field is replaced, the spin on the other end of this rung has only two nearest neighbors, so it can be rotated with the formation of two domain wall-like structures symmetric about the impurity. In the other situation when an antiparallel spin is replaced this type of structure appears to be unfavorable and the localized state is absent. These two situations can be combined to understand why the localized state only appears on one side of the two impurities, namely, the side with the parallel spin replaced will exhibit the nonuniform state and the side with the anitparallel spin replaced will be uniform above the bulk spin flop transition.

This work was supported by National Science Foundation Grant No. DMR-9974273.

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