Non-Degenerate Ground State in the Antiferromagnetic Double-Exchange Model on a Triangular Lattice.

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In order to study effects of frustration in an itinerant electron system, we investigate ground states of the antiferromagnetic double-exchange model on a triangular lattice. In this model, pseudo-spins are coupled to electron transfer integrals in such a way that antiparallel configurations of pseudo-spins gain kinetic energies. Although the antiferromagnetic Ising model on a triangular lattice shows macroscopic degenerate ground states, the present model shows that the degeneracy is lifted due to long-range natures of the double exchange interactions. Spin ordering at the ground state is also discussed.

KEYWORDS: antiferromagnetic double-exchange model, triangular lattice, geometrical frustration, degeneracy

One of the interests in the study of frustrated systems is to investigate anomalous ground states where conventional long-range orders are suppressed. In some systems, disordered ground states with macroscopic degeneracies are observed. Since such states are thermodynamically unstable, singular responses to perturbations may be observed. Typical examples are antiferromagnetic (AF) Ising models on geometrically frustrated lattices, e.g., on triangular, kagomé, and pyrochlore lattices.

Another example which shows the macroscopically degeneracy is the spin ice system on kagomé and pyrochlore lattices. In these systems, spins have uniaxial anisotropies so that they take either of "inward" and "outward" states. We define the pseudo-spin \( \tilde{s}_i \) by \( \tilde{s}_i = 1 \) (1) if the spin on the \( i \)-th site points outward (inward). In spin ice systems, ferromagnetic interaction between spins can be mapped to AF interaction between pseudo-spins. Therefore, the spin ice model with ferromagnetic nearest neighbor (n.n.) Ising interactions exhibits macroscopically degenerate ground states.

When such macroscopic degeneracies are lifted by residual interactions, peculiar states such as cluster ordered states emerge as the ground states. For instance, when dipolar long-range interactions are introduced in the spin ice model on a pyrochlore lattice, a spin cluster ordered state is observed at sufficiently low temperatures.

Recently, the authors have investigated frustrated itinerant electron systems. One of the
motivation to investigate such systems is to study anomalous ground states which might exhibit unconventional transport and optical properties. Another interesting point is to understand how the nature of interactions in itinerant electron systems are different from those in localized spin systems. We have introduced a double exchange spin ice (DESI) model in the strong Hund's coupling limit on a kagome lattice, and observed a spin cluster ordered state which is named the dodecam er ordered phase. In the DESI system, interactions are ferromagnetic due to the double exchange mechanism, and uniaxial anisotropies are introduced for local spins. Due to the spin ice mechanism, there exist AF interactions between the pseudo-spins defined on the kagome lattice. The DESI model exhibits a translational symmetry broken state, although the analogous spin ice system has disordered ground state with the macroscopic degeneracy. Thus, differences in the nature of interactions make qualitatively different results in the behaviors of the ground states.

The realization of the spin ice mechanism enables us to construct a double exchange system with the AF interaction between pseudo-spins. It is difficult to introduce such mechanisms on geometrically frustrated lattices other than the kagome and the pyrochlore lattice. However, in order to investigate the effects of the kinetics of electrons and the frustration, let us simply extend them model to general cases on various frustrated lattices. We define an antiferromagnetic double-exchange (AF-DE) model in the form,

$$H^F = \sum_{i<j} t(i,j) \sigma_i^+ \sigma_j + h \sigma_i^z;$$  \hspace{1cm} (1)

where the summation is taken over all pairs of the n.n. sites, and

$$t(i,j) = \begin{cases} t & (i = j); \\ t^0 & (i \neq j). \end{cases}$$  \hspace{1cm} (2)

Here, \(t\) and \(t^0\) are strong and weak transfer integrals, respectively, which satisfies \(t^0 = t \leq t = 1\).

It is easily found that the AF-DE model on a geometrically frustrated lattice is a frustrated electron system.

The DESI model corresponds to the AF-DE model on a kagome lattice with \(t^0 = t = 1\). For a given spin configuration, the energy of the AF Ising model is determined by the number of AF bonds, \(N_{AF}\). Similarly, in the AF-DE model, \(N_{AF}\) gives the total number of strong-hopping bonds. Increase of \(N_{AF}\) roughly gives the kinetic energy gain. Therefore, there exist AF interactions between pseudo-spins in the AF-DE model. To be precise, however, pseudo-spin interactions in the AF-DE model are not identical to those in the AF Ising model. The energy of the AF-DE model for a given pseudo-spin configuration \(f \sigma_i\) is given by

$$E_K (f \sigma_i) = \sum_{i<j} t(i,j) \sigma_i^+ \sigma_j + h \sigma_i^z;$$  \hspace{1cm} (3)

where \(h \sigma_i^z\) represents an expectation value at the ground state. If \(h \sigma_i^z\) is constant, \(E_K\)
depends only on \( N_{AF} \) so that the AF-DE model can be mapped to the AF Ising model exactly. However, this is not the case, since the expectation value of electron hopping \( h \hat{c}_j^\dagger \hat{c}_j + h \hat{x}_i \hat{x}_0 \) depends on both eigenenergies and wavefunctions of the Hamiltonian. Due to the extended nature of the wavefunctions of the itinerant electrons, \( h \hat{c}_j^\dagger \hat{c}_j + h \hat{x}_i \hat{x}_0 \) cannot be expressed by local pseudo-spin configurations in a simple manner. Namely, a change in a pseudo-spin on the \( k \)-th site \( \hat{s}_k \) affects the wavefunctions and hence \( h \hat{c}_j^\dagger \hat{c}_j + h \hat{x}_i \hat{x}_0 \) in neighboring sites. Therefore, \( E_K \) depends on the global lattice structure which consists of strong and weak bonds. As a result, behaviors of the AF-DE model at low temperatures might be different from those of the AF Ising model.

In this paper, in order to investigate non-trivial ground states in the frustrated itinerant electron systems, the AF-DE model on the triangular lattice is studied. For simplicity, we take \( t^0 = 0 \) throughout this paper. We also set the chemical potential \( \mu = 0 \). Results for \( t^0 \neq 0 \) will be reported elsewhere.

![AF chain stacked state](image)

Fig. 1. An AF chain stacked state of the AF Ising model, where each AF chain is indicated by arrows.

Open and closed circles represent the up- and the down-spins, respectively. Solid lines represent bonds with AF configuration, while dashed lines represent bonds with ferromagnetic configuration.

The ground states in the AF Ising model which maximize \( N_{AF} \) may be considered as good candidates for those in the AF-DE model. Among all ground states in the AF Ising model, two types of them are shown in Fig. 1 and Fig. 2. One is a state constructed by stacking the AF chains (AF chain stacked state) [Fig. 1], and the other is one which has the three sublattice structure [Fig. 2(a)], i.e., the up-spin sublattice, the down-spin sublattice and the A sublattice. As shown in Fig. 2(b), each spin state on the A sublattice can be determined independently since \( N_{AF} \) does not depend on spin states on A sublattice. Hereafter, we treat the AF-chain stacked states and the three sublattice states as the possible candidates for the ground state in the AF-DE model and calculate energies of these states for small systems.

In order to check whether the degeneracy in the Ising system can be lifted by the kinetics of electrons in the AF-DE model or not, we have calculated energies of the AF chain stacked states and the three sublattice states for the finite system sizes. In order to extrapolate the energy
Fig. 2. Three sublattice structure in the AF Ising model. Open and closed circles represent the up- and the down-spins, respectively. (a) Lattice sites consist of three sublattices, "up-spin", "down-spin" and "A" sublattices. Directions of spins on A sublattice sites are arbitrary. (b) An example of the three sublattice structures. Solid lines represent bonds with AF configuration, while dashed lines represent bonds with ferromagnetic configuration. A sublattice sites are indicated by dashed circles. \( N_{AF} \) does not depend on the spin states on the A sublattice since such spins always have three up-spins and three down-spins at n.n. six sites.

Fig. 3. AF chain stacked states in the AF-D E model. Open and closed circles represent the up- and the down-spins, respectively. Solid lines represent bonds created by the electron hopping. The patterns (b) and (c) are obtained from the pattern (a) by hopping the AF chain indicated by the arrows. In terms of the electron hopping, these patterns are topologically identical to the regular square lattice (d), although spin configurations are different from each other.

in the thermodynamic limit from that in the finite system, twisted boundary conditions have been applied, and the energy of the system has been calculated by averaging over phases. This procedure extrapolates the energy to that for a system in the thermodynamic limit with a finite-sized supercell. The density of states (DOS) in each spin configuration has also been calculated by this method.

First, let us discuss the AF chain stacked states in the AF-D E model. Considering the
electron hopping, it is found that the degeneracy in the AF chain stacked state cannot be lifted as follows. Since electrons can only hop between the up- and the down-spins, the AF chain stacked states can effectively be mapped to an electron system on a lattice which is created by disconnecting ferromagnetic bonds. Several AF chain stacked states in the AF-DE model are shown in Fig. 3. For example, the spin configuration in Fig. 3(b) is obtained from that in Fig. 3(a) by flipping the AF chain indicated by the arrow. Other configurations [e.g., Fig. 3(c)] can be obtained in the same manners. Although spin configurations are different from each other, these AF chain stacked states are topologically equivalent to the square lattice as long as the electron hoppings are concerned [see Fig. 3(d)]. In this way, in the thermodynamic limit, all AF chain stacked states are regarded as the identical square lattice, and thus, have the same energy.

Next, we consider the three sublattice states. The energy of all possible spin configurations within the three sublattice states which consist of supercells with 6 6 sites in the thermodynamic limit (6 6 supercells) has been calculated. Note that there exist 2^{12} configurations for A sublattice spins in this case. As a result, we have found that the degeneracy is lifted by the kinetics of electrons. The smallest energy state with the 6 6 supercell in the thermodynamic limit is shown in Fig. 4. Such a periodic state is determined uniquely except for the trivial degeneracy. Concerning electron hopping, each spin configuration in the three sublattice states can be mapped to a certain lattice different from each other. It is natural that the degeneracy in the three sublattice state is lifted by the electron motions, since the kinetic energy of electrons is strongly dependent on the path of electrons.

Let us consider which state, the AF chain stacked state or the three sublattice state, is energetically stable. Numerical calculation shows that the smallest energy state in the three sublattice states is more stable than the AF chain stacked states. The energy per site for the AF chain stacked states and that for the three sublattice states are -0.811t and -0.813t,
Fig. 5. (a) Density of states (DOS) of the square lattice. (b) DOS of the most stable state in the three sublattice states with the $6 \times 6$ supercell in the thermodynamic limit.

respectively. The DOS of the AF chain stacked states and that of the most stable three sublattice state are shown in Fig. 5(a) and Fig. 5(b). In Fig. 5(b), we find several dips or imperfect gaps. It is considered that such dips are ascribed to the periodic spin structure, that is, the band gap is partially opened by the breaking of the translational symmetry. On the other hand, any gaps have not been observed in the case of the AF chain stacked states in Fig. 5(a). Thus, the three sublattice state is expected to be stabilized by the gap opening due to the appearance of a certain periodicity.

As mentioned previously, in the AF Ising model, the ground state is determined by maximizing $N_{AF}$, while it is quite plausible but still not certain whether the ground state of the AF-DE model has the maximum number of $N_{AF}$. In order to search the ground state in the AF-DE model on the triangular lattice, energies of all possible spin configurations for small
system with 3 3 and 4 4 supercells in the thermodynamic limit have been calculated. As a result, it is found that any spin configurations except for the AF chain stacked states and the three sublattice states cannot be stabilized. It seems that the ground state has the maximum number of $N_{AF}$ also in the AF-DE model.

Throughout this paper, two types of the ground states in the AF Ising model have been considered, i.e., the AF-chain stacked states and the three sublattice states, as the possible candidates for the ground state of the AF-DE model. As far as we have searched the lowest energy state among such two kinds of states for small system sizes when $t^0 = 0$ and $\alpha = 0$, it is found that the ground state is selected from the three sublattice states. Such a ground state might also be affected by $\alpha$. The DOS shown in Fig. 5(b) has the largest dip around $\alpha = 0$, which may stabilize the ground state shown in Fig. 4. Changing $\alpha$ in the AF-DE system, other periodic patterns in the three sublattice states can emerge as the ground state by opening the gap around $\alpha = 0$. On the other hand, it is considered that the stability of the AF chain stacked states does not depend on $\alpha$. Thus, at least two possibilities are considered: (1) The ground states with commensurate periodic structures can be realized only at a certain $\alpha$, and otherwise, the AF chain stacked states appear in the ground states with degeneracy. (2) At each $\alpha$, ground states with possible incommensurate periodicities corresponding to are selected from the three sublattice states, and thus, the ground state does not have the degeneracy in all range. More detailed analyses are needed to clarify this point.

In conclusion, as far as the AF-chain stacked states and the three sublattice states are considered, the lowest energy state for the system with 6 6 supercells can be selected uniquely from the latter states. Thus, degenerate ground states in the AF Ising model can be lifted by the effect of motions of electrons in the AF-DE model. In this way, according to the nature of the interaction, the ground state is drastically changed. In the frustrated electron system, the kinetics of electrons plays an important role to lift the degeneracy due to the frustration and possibly leads to an ordered state.
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