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Quantitatively microscopic interpretations on magnetization-plateau phenomena in stacked triangular Ising antiferromagnets

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ABSTRACT

A Monte Carlo method based on zero-temperature Glauber algorithm is employed to study field-induced magnetization-plateau behaviors in frustrated Ising antiferromagnets on stacked triangular lattices. The plateau heights and transitions are strongly dependent on ratios of interlayer to intralayer exchange constant. All the macroscopic phenomena have been quantitatively interpreted by means of microscopic spin orientations and evolutions. The same magnitude of exchange constants throughout the system opens new avenues along the stacking directions to spread intralayer frustration effects and to induce more active spin reversals. Accurate correspondence is also established, not only used to predict all the plateau transitions and heights but also to interpret the zero-field remanent magnetization as well as the magnetically hysteretic phenomena unambiguously.

1. Introduction

Ising antiferromagnets on stacked triangular lattices (IASTL) could exhibit two ordered phases at different temperatures (T), which were both six-fold degenerate and accommodated order and disorder on three interpenetrating sublattices, and have been studied extensively for a long time [1,2]. Netz and Nihat Berker combining mean-field and Monte Carlo (MC) approaches obtained an accurate phase diagram of IASTL, accessible to experiments [3]. Plumer et al. also studied the magnetic field (h)–T phase diagram of IASTL using extensive histogram MC simulations, and presented that the transition from period-3 ordered state to paramagnetic phase remained in the XY universality class [4,5]. Recently, Žukovič and his colleagues explored the influences of T and ferromagnetic exchange interaction in the stacking direction on the magnetization processes in IASTL and observed that the new plateaus only appeared at sufficiently low T and sufficiently large interlayer couplings [6]. More significantly, one has suggested that the three-dimensional IASTL models with appropriate interactions are used to simulate real one-dimensional spin-chain compounds and reproduce many fascinating T/time-dependent multistep magnetization behaviors [7–12].

Although there have been considerable theoretical efforts in the frame of IASTL on the studies of the origin of multiple magnetization-plateau behaviors at low T, some unanswered questions are still left over: (i) degree of one-dimensionality has not been unambiguously established experimentally, and the role of interlayer coupling in the magnetization plateaus needs to be explored further; (ii) how to generate the hysteretic behavior between field-decreasing (FD) and field-increasing (FI) processes as well as the resultant plateau shift and spin evolution has not been demonstrated; (iii) whether the height is randomly formed on each plateau is also not elucidated. It would, therefore, be interesting to solve the issues in this paper. We exploit the simplest IASTL model and employ a MC method based on zero-T Glauber algorithm to investigate h-driven multiple magnetization-plateau phenomena and magnetically hysteretic behaviors. Finally, the plateau and hysteresis as well as zero-field remanence phenomena are not only well interpreted quantitatively, but also we can successfully predict all the plateau transitions and calculate all the plateau positions.

2. Model and Monte Carlo simulation

Two-monolayer rhombic 120×120 supercells of the triangular lattices with periodic boundary conditions are chosen, although few periodic structures can appear during the simulation. To avoid artificial domain boundaries the length of supercell should be a multiple of periodicity of these structures [13], meanwhile, preliminary calculations on supercells with several sizes showed a good convergence of the results. The Hamiltonian is given by

$$\mathcal{H} = -J \sum_{<ij>} \mathbf{S_i} \cdot \mathbf{S_j} - J' \sum_{<ik>} \mathbf{S_i} \cdot \mathbf{S_k} - h \sum_i \mathbf{S_i}, \quad (1)$$

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where the spin **S**, labeled by its site indices *i*, *j*, and *k*, is classical and as a discrete Ising-model spin ($S=\pm1$), agreeable with some experimental findings on relevant materials [14]. The first two terms denote the intralayer and interlayer nearest-neighbor exchange interactions, respectively. The intralayer exchange constant $J=-1.0$ is as a fixed unit quantity to reduce other parameters, while the interlayer one J' is varied between −2.0 and 2.0 to study its role in magnetization behaviors, which means that the fully frustrated three-dimensional systems and the intralayer frustrated systems with no competing interactions in the stacking directions are both considered. Finally, a Zeeman energy term, where h is applied along the stacking directions, must also be included and this external polarization adds another degree of complexity to the interplay between the first two energy terms [15]. For different real materials, S, J, and J' should have different concrete values. Although their real values are not available from experiments, a reasonable choice of them is judged from a quantitative comparison between simulation results and experimental data. It is noteworthy that the dipolar interactions which should be present in nanowires and other low-dimensional systems are not taken into account here, because their overall effect is merely to induce an effective antiferromagnetic field that retards h at which the plateaus occur [16].

In this paper, we focus on the low-T magnetization behaviors in the geometrically frustrated systems, and if T is very low, it is difficult for the thermal fluctuation to overcome the energy barriers between metastable states and ground states. The system cannot relax into the ground state in a finite amount of time and is frozen into the metastable state. Accordingly, the Glauber algorithm, as a well-accepted rule which ignores the thermal fluctuations while allows the random fluctuations of spins at $T=0$ [13,17–20], is employed to scrutinize the microscopic spin configurations and to explore the metastable states. This approach is a frozen metastability approximation and excludes quantum dynamical effects, because the magnetic system is assumed to lose the coherence during very long relaxation times and the quantum correlations are destroyed, consistent with realistic statistical systems [13,18].

The simulation starts from a strong h of 10.0 and the IASTL system with an ordered parallel configuration along the stacking directions to avoid the results obtained coincidentally as a result of a particular random initialization. Then h decreases to zero and immediately increases back to the initial value in steps of $\Delta h=0.05$ without any interval, and thus a magnetizing loop is formed. The evolution time (t) is measured by MC steps and a complete magnetization-h loop would cost totally $t=8.02\times10^6$ MC steps per spin. This sweep rate is slow enough to guarantee quasiequilibrium.

3. Results and discussion

Fig. 1 indicates the FD and FI magnetization behaviors in the IASTL with different ratios of J'/J. When $|J'/J|$ is not equal to 1.0, three magnetization plateaus are observed and their heights are 1.0, 0.5, and 0.0. Additionally, two minor hysteresis loops emerge simultaneously if J' is ferromagnetic and the loop widths are approximately equal to $2|J'/J|$. On the contrary, no hysteretic behaviors appear for the case of antiferromagnetic J' while the critical h values where the plateau transitions occur are also proportional to J'/J and shift towards lower values. However, some novel results are obtained as $|J'/J|=1.0$. Firstly, more hysteretic phenomena appear. It is well-known that magnetically hysteretic phenomena are related to quasiequilibrium states, i.e., related to the states in which the systems under consideration are trapped

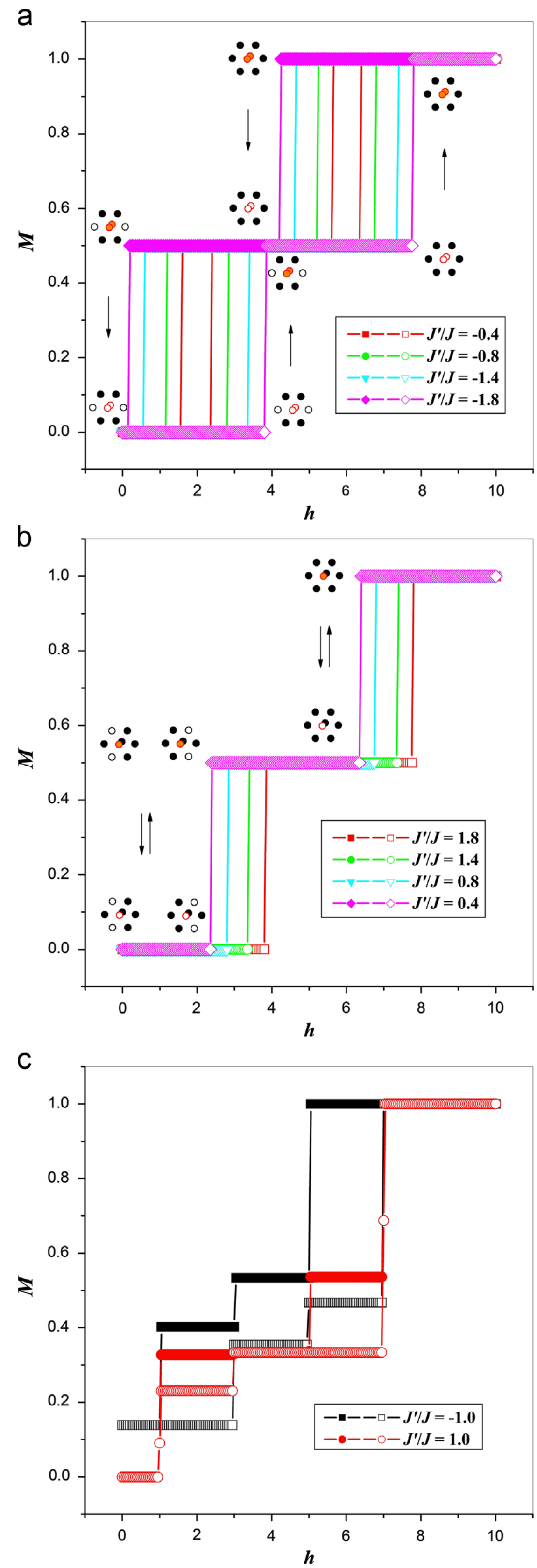

Fig. 1. (Color online) Field-decreasing (solid symbols) and field-increasing (open symbols) magnetization behaviors in the IASTL with different ratios of J'/J. Orange dots inserted denote the rotatable spins when the plateau transitions occur, black and white ones denote their up and down nearest-neighbor intralayer and interlayer spins, and arrows describe the evolutions of spin reversals.