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The expanded triangular Kitaev–Heisenberg model in the full parameter space

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ABSTRACT

The classical Kitaev–Heisenberg model on the triangular lattice is investigated by simulation in its full parameter space together with the next-nearest neighboring Heisenberg interaction or the single-ion anisotropy. The variation of the system is demonstrated directly by the joint density of states (DOS) depending on energy and magnetization obtained from Wang–Landau algorithm. The Metropolis Monte Carlo simulation and the zero-temperature Glauber dynamics are performed to show the internal energy, the correlation functions and spin configurations at zero temperature. It is revealed that two types of DOS (U and inverse U) divide the whole parameter range into two main parts with antiferromagnetic and ferromagnetic features respectively. In the parameter range of U type DOS, the mixed frustration from the triangular geometry and the Kitaev interaction produces rich phases, which are influenced in different ways by the next-nearest neighboring Heisenberg interaction and the single-ion anisotropy.

1. Introduction

The spin–orbital coupling has been much highlighted in recent years due to its key role in the condensed matter physics, especially for the topological band insulators [1,2]. It is expected that the materials containing the heavy elements with large spin–orbit coupling may provide a fertile ground to search for topological insulators. Among them, the oxides group of transition metal Ir attracts considerable attention. In these compounds, the spin–orbit coupling and orbital degeneracy could make the exchange interaction highly anisotropic and frustrated, giving rise to realization of exotic spin models. In particular, the Kitaev–Heisenberg model has been proposed to capture the magnetic interactions in the honeycomb iridates [3–8]. Since the intrinsic spin–orbit coupling substantially modifies the effective spin Hamiltonian, the novel topological states are possible to arise in such systems, which has been another subject of intense interest [9,10].

Beyond the highlighted honeycomb lattice, other geometries, which could be built from edge-sharing IrO_6 octahedra and thus also could host the Kitaev–Heisenberg physics, provide a rich playground for exotic phenomena [5]. For example, Z_2-vortex lattice has been observed in the ground state of the triangular Kitaev–Heisenberg model [11]. Thus, the Kitaev–Heisenberg model on other structures has become a new attraction recently. On the other hand, differently from the conventional Kitaev–Heisenberg model with the Kitaev interaction between the nearest neighboring spins on the honeycomb lattice, more recent investigations show that the Kitaev interaction can also appear between the next-nearest neighboring spins [12,13]. Such a honeycomb lattice can be regarded as two interpenetrating triangular Kitaev–Heisenberg sublattices connected by the nearest neighboring bonds [11]. Therefore, the investigation on the triangular Kitaev–Heisenberg model will help to understand the honeycomb iridates.

In this Letter, Monte Carlo simulation is performed to investigate the Kitaev–Heisenberg model on the triangular lattice expanded to its full parameter space. The character of the system is demonstrated directly by the density of states (DOS). Two types of DOS (U and inverse U (IU)) divide the whole parameter range into two main parts (U region and IU region) together with the transition regions between them. Rich phases at low temperature (T) are observed in the U region, which are induced by the mixed frustration from the triangular geometry and the Kitaev interaction. Moreover, the triangular Kitaev–Heisenberg model is further expanded to include more terms usual in materials. It is revealed that the next-nearest neighboring Heisenberg interaction has effect on the ranges of the U and IU regions and the corresponding low-temperature (low-T) phases. The single-ion anisotropy hardly influences these ranges, although it modifies the shape of DOS.

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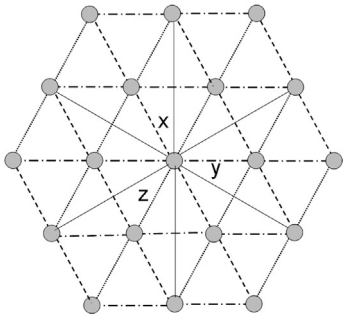

Fig. 1. A sketch of the triangular lattice. The dashed, dotted-dashed and dotted links indicate the nearest neighboring spin-dependent bonds, where x, y and z involve S^x, S^y, and S^z respectively. The solid thin line represents the next-nearest neighboring bonds.

2. Model and simulation

In the triangular Kitaev–Heisenberg model, the exotic Kitaev interaction brings an unconventional frustration into the triangular structure with the conventional geometric frustration, forming a mixed frustrated system. Note that one character of frustration is a high degeneracy of ground states and plenty of metastable states. Wang–Landau (WL) algorithm, which can avoid the system getting stuck in the metastable states and has a straightforward connection with DOS, had been applied in the investigation of frustrated systems efficiently [14–16]. We take its advantage to calculate DOS directly [17,18].

We consider a classical Kitaev–Heisenberg spin model on the two-dimensional triangular lattice. Similar to the Hamiltonian of the Kitaev–Heisenberg model on the honeycomb lattice [4,7], the energy (E) can be written as

$$E = J_H \sum_{\langle i,j\rangle} S_i \cdot S_j + J_K \sum_{\langle\gamma\rangle} S_i^{\gamma} \cdot S_j^{\gamma} + J_N \sum_{\langle\langle i,k\rangle\rangle} S_i \cdot S_k + D \sum_i \left(S_i^z\right)^2, \tag{1}$$

where S_i denotes the effective spin with unit magnitude. J_H is an isotropic Heisenberg coupling between spins on the nearest neighboring sites ($\langle i, j\rangle$) of the triangular lattice. The Kitaev interaction J_K couples the γ-component of spins ($\gamma = x, y$ and z) on the γ-links between the nearest neighboring spins as plotted in Fig. 1. J_N is a Heisenberg interaction between spins on the next-nearest neighboring sites ($\langle\langle i, k\rangle\rangle$), and the last term represents the single-ion anisotropy along z-axis with the strength D.

Following the WL algorithm, a joint DOS ($g(E, M)$) is accumulated by the random walk carried out in the energy and magnetization (E&M) space, where M denotes the magnetization evaluated in the direction of *z-axis*, namely

$$M = \sum_i S_i^z \tag{2}$$

In the continuous E&M space, E and M are discretized by introducing bins of $\Delta E = 0.25$ and $\Delta M = 0.25$ [19,20]. To overcome the difficulty of dealing with the boundaries of the accessible conformational space and avoiding the calculation process trapped in these regions without being able to escape, at the beginning of simulation, a preliminary calculation is run to delimit the practical range of available states [21]. During this initial procedure, a bin is marked as accessible state once it is visited, and the total number of visited bins is ensured to show a saturation behavior. After that, the standard WL algorithm is carried out by simply ignoring those bins outside of the determined domain of available states [22]. We reduce the modification factor (f) according to the recipe $f_{i+1} = f_i^{1/2}$ until the final modification factor reaches $f_{\text{final}} = 1.0000019$. For every f, the histogram for all possible E and M is required not less than 80% of the averaged histogram. The WL simulation is performed on an $L \times L$ triangular lattice ($L = 6$ and the total number of spins $N = 36$) with period-boundary conditions assumed. To confirm the results of $L = 6$, the lattice of $L = 12$ is also simulated on some parameter points, and the DOSs obtained show the same character.

By parameterizing $J_H = \cos\varphi$ and $J_K = \sin\varphi$, the ratio of J_H to J_K is considered to its whole range by scanning φ from 0 to 2π. Noting that the parameters have the same values at $\varphi = 0$ and 2π, the range $[0, 2\pi]$ actually forms a parameter ring. To give a better comparison between DOSs on different parameter points, based on the DOS obtained, we extract the E&M map which is the profile of DOS on E&M plane, showing all the possible states in the E&M space. Moreover, we calculate the density of states as a function of E (EDOS), i.e. $g(E)$, which is obtained by cumulating $g(E, M)$ of different M at every E point.

On the other hand, the Metropolis Monte Carlo simulation and the zero-temperature Glauber dynamics (MG) are applied to present spin configuration directly. At first, the system is evolved by Metropolis algorithm from a relatively high T to a very low T gradually, and then the zero-temperature Glauber dynamics is applied to reduce the energy of the system as low as possible. Based on the state with the lowest E, the correlation on the nearest neighboring spins (C_n) and that on the next-nearest neighboring spins (C_{nn}) are calculated in the forms of

$$C_n = \langle S_i \cdot S_{i+1}\rangle_n \tag{3}$$

$$C_{nn} = \langle S_i \cdot S_{i+2}\rangle_{nn} \tag{4}$$

The MG simulation is performed on the triangular lattice of $L = 24, 36$ and 48. All the data with different lattice sizes coincide with each other.

3. Results and discussion

3.1. The pure Kitaev–Heisenberg model ($J_N = 0$ and $D = 0$)

Without the next-nearest neighboring interaction and the single-ion anisotropy, the DOSs obtained from WL simulation are plotted in Fig. 2 partially. There are two Heisenberg points at $\varphi = 0$ and π with $J_K = 0$, corresponding to the conventional triangular systems with the pure antiferromagnetic (AFM) and ferromagnetic (FM) interactions, where the DOSs in the U and inverse U (IU) shapes are observed respectively (Figs. 2(a) and 2(i)). Between these two Heisenberg points on the parameter ring, the DOS shows a continuous variation by the modulation of the interaction ratio, and two shapes of DOS (U and IU types) dominate on the whole range of φ. It is noteworthy that all the DOSs have two sharp corners with the largest $|M/N| = 1$, which correspond to two particular FM states with all the spins aligned along z-axis (zFM states). In the case of IU type, the two zFM states with the lowest E degenerate with other FM states (with its magnetization not aligned along z-axis) on the bottom line, which indicates that the dominate interaction is FM. On the contrast, in the case of U type, zFM states have the highest energy, which means AFM interaction dominates. Between the U and IU types, there are transition shapes as shown in Figs. 2(f) and 2(n), where the competition between the Heisenberg interaction and Kitaev one induces an intermediate energy to the zFM states.

In Fig. 2, it is interesting to note that the second row looks just like the reflection of the first row. The reason is that on the condition of $J_N = 0$ and $D = 0$, when the difference of φ is π, both J_H and J_K change their sign, and hence the whole Hamiltonian changes its sign. Therefore, the DOS is inversed as a whole.