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Zigzag order and phase competition in expanded Kitaev–Heisenberg model on honeycomb lattice

Xiaoyan Yao *

Department of Physics, Southeast University, Nanjing 211189, China

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ABSTRACT

The Kitaev–Heisenberg model on the honeycomb lattice is investigated in two cases: (I) with the Kitaev interaction between the nearest neighbors, and (II) with the Kitaev interaction between the next nearest neighbors. In the full parameter range, the ground states are searched by Monte Carlo simulation and identified by evaluating the correlation functions. The energies of different phases are calculated and compared with the simulated result to show the phase competition. It is observed from both energy calculation and the density of states that the zigzag order shows a symmetric behavior to the stripy phase in the pure Kitaev–Heisenberg model. By considering more interactions in both cases, the energy of zigzag order can be reduced lower than the energies of other states. Thus the zigzag phase may be stabilized in more parameter region and even extended to the whole parameter range.

1. Introduction

Iridates were much highlighted in recent years since they were suggested as promising candidate materials for the topological band insulators [1–3]. For hexagonal iridates with general formula A_2IrO_3 (A = Na, Li), the spin–orbit coupling and orbital degeneracy could make the exchange interaction highly anisotropic and frustrated. The entangled spin and orbital states break the SU(2) symmetry of the magnetic Hamiltonian, giving rise to realization of exotic spin models. In particular, the Kitaev–Heisenberg (KH) model as follows has been proposed to capture the magnetic interactions in the honeycomb iridates [4–6].

$$H = J_{Hn} \sum_{\langle i,j\rangle} S_i \cdot S_j + J_{Kn} \sum_{\langle i,j\rangle_\gamma} S_i^\gamma \cdot S_j^\gamma \tag{1}$$

where J_{Hn} is an isotropic Heisenberg coupling between spins (S_i and S_j) on the nearest-neighboring sites ($\langle i, j\rangle$). J_{Kn} is a Kitaev interaction, coupling different spin components (S^x, S^y, and S^z) on the nearest-neighboring bonds along the three lattice directions, where $\gamma = x$, y and z labels the direction of the bonds as plotted in Fig. 1(a). The original version of this nearest-neighboring Kitaev–Heisenberg (NKH) model with antiferromagnetic (AFM) J_{Hn} and ferromagnetic (FM) J_{Kn} presents a spin-liquid state near the Kitaev limit, a Néel order close to the Heisenberg limit and a stripy phase between them [5,7,8].

However, the experiments of iridates soon brought a surprising challenge to this attractive model. A resonant x-ray scattering measurement on Na_2IrO_3 found the evidence of unconventional magnetic order at low temperature which showed magnetic Bragg peaks at wave vectors consistent with either a stripy or a zigzag order. Combining the experimental data with the first-principles calculations, the most likely spin structure in the ground state was proposed to be the zigzag structure [9]. Then this conclusion was verified independently by using inelastic neutron scattering and single-crystal neutron diffraction [10,11]. Thus, the zigzag phase, which is missed in the original version of the NKH model mentioned above, came to the focus. To resolve this problem, one effective modification is to extend the original NKH model to its full parameter space by considering additional hopping processes based on the interorbital t_{2g}–e_g hopping. Then the zigzag order was found in a previously overlooked parameter range with an FM J_{Hn} and an AFM J_{Kn} [12,13]. Another successful modification is to include farther interactions beyond the nearest-neighboring exchange. It was shown on both classic and quantum levels that the zigzag magnetic order may be stabilized by including substantial second- and third-nearest-neighboring AFM interactions [14,15].

In addition, different from the NKH model with the Kitaev interaction between the nearest-neighboring spins on the honeycomb lattice, the recent investigations showed that the Kitaev interaction can also appear between the next-nearest-neighboring spins (Fig. 1(b)), namely the next-nearest-neighboring Kitaev–Heisenberg (NNKH) model, which was obtained in the strong interaction limit of a Hubbard model on the honeycomb lattice.

* Tel.: +86 25 52090606 8301; fax: +86 25 52090600 8204.
E-mail address: yaoxiaoyan@gmail.com.

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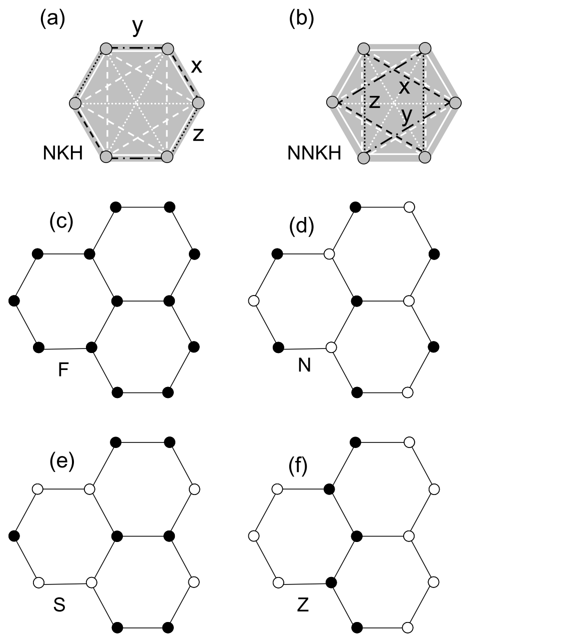

Fig. 1. Sketches of the honeycomb lattice for (a) the NKH model and (b) the NNKH model. The solid, dashed and dotted white links indicate the nearest-, second-nearest- and third-nearest-neighboring bonds. The dashed, dot-dashed and dotted black links indicate three kinds of spin-dependent bonds for (a) the nearest-neighbors and (b) the next nearest-neighbors. Sketches of the typical spin structures for (c) F, (d) N, (e) S and (f) Z phases. Open and filled circles correspond to up and down directions of spins.

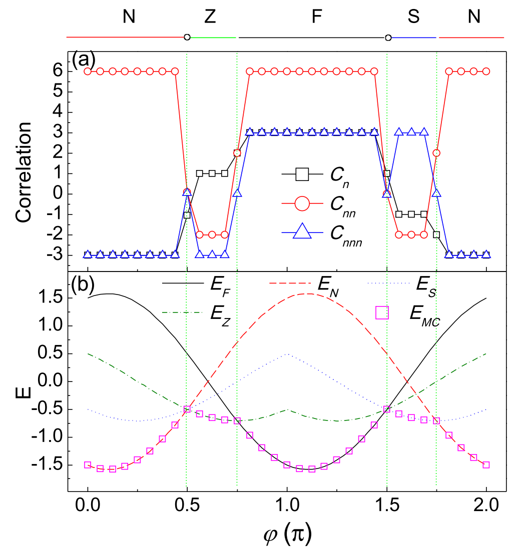

Fig. 2. (Color online) The pure NKH model with $J_{Hnn} = 0$ and $J_{Hnnn} = 0$. (a) The correlation functions C_n, C_{nn} and C_{nnn} as functions of φ. The four dominant phases F, N, S and Z can be identified as shown on the top, where two empty circles represent the spin liquid states. (b) The φ-dependences of the classic energies per site of F, N, S and Z phases, namely E_F, E_N, E_S and E_Z. The squares show the energies of the ground states obtained from MC simulation (E_{MC}).

Here the ground state with stripy order was revealed to possess some degree of zigzag order [16,17].

Although some efforts have been made, the zigzag order, as an important key for the KH model to connect with experiments of iridates, still remains controversial up to now. In present work, both the NKH and NNKH models are investigated to the full parameter space to explore the zigzag order and the phase competition in these systems. In the pure NKH model there are four dominant collinear magnetic phases, namely ferromagnetic (F), Néel (N), stripy (S) and zigzag (Z) phases. The symmetric behavior is observed between them. Especially for Z and S phases, the symmetric behavior is also reflected on the density of states (DOS). By the energy calculation, the competition between the dominant magnetic phases is discussed in detail. It is revealed that to enhance Z phase is to lower the energy of Z order and to suppress other phases, which can be realized by considering more neighboring Heisenberg interactions in both NKH and NNKH models.

2. Simulation and calculation

To explore the possible ground state on every parameter point, the Monte Carlo (MC) simulation is performed on a honeycomb lattice of $N = 1536$ sites with periodic boundary conditions applied. The system is first evolved by the Metropolis algorithm from a relatively high temperature to a very low temperature gradually. Then, in order to reach the limit of zero temperature, the minimization algorithm for energy (E), namely only the proposed update with the energy variation not higher than zero can be accepted, is applied to further push the system to the ground state. The final result is obtained by comparing independent data sets evolving from different initial states. Based on the ground state obtained, the correlation functions on the nearest-neighboring spins (C_n), on the second-nearest-neighboring spins (C_{nn}) and on the third-nearest-neighboring spins (C_{nnn}) are calculated in the forms of

$$C_n = \langle S_i \cdot S_{i+1} \rangle_n \tag{2}$$

$$C_{nn} = \langle S_i \cdot S_{i+2} \rangle_{nn} \tag{3}$$

$$C_{nnn} = \langle S_i \cdot S_{i+3} \rangle_{nnn} \tag{4}$$

On the other hand, as a supplement, the DOS in energy and magnetization ($E\&M$) space is evaluated by performing Wang–Landau (WL) simulation on a honeycomb lattice of $N = 24$ spins with periodic boundary conditions assumed, where M denotes the magnetization in the direction of *z-axis*. The continuous $E\&M$ space is discretized by introducing bins of $\Delta E = 0.25$ and $\Delta M = 0.25$ [18,19]. At the beginning of simulation, a preliminary calculation of WL algorithm is run to delimit the practical scope of available states [20]. Then the standard WL algorithm is carried out by simply ignoring those bins outside of the determined domain of available states [21]. We reduce the modification factor (f) according to the recipe $f_{i+1} = f_i^{1/2}$ till the final modification factor reaches $f_{\mathrm{final}} = 1.0000019$. For every f, the histogram for all possible E and M is required not less than 80% of the averaged histogram. To give a better comparison between DOSs on different parameter points, we extract the $E\&M$ map from the DOS obtained, which is the profile of DOS on $E\&M$ plane, showing the boundary of all the possible states in the $E\&M$ space [22].

3. Results and discussion

3.1. The NKH model extended to full parameter range

First, the pure NKH model of Eq. (1) is simulated in the parameter space of J_{Hn} and J_{Kn}, which is extended in a symmetric way by parameterizing $J_{Hn} = \cos\varphi$ and $J_{Kn} = \sin\varphi$. The ratio of J_{Hn} to J_{Kn} is considered to its whole range by scanning φ from 0 to 2π. Based on the ground states obtained from MC simulation, the correlation functions show four distinct ranges as plotted in Fig. 2(a), in which four collinear magnetic phases can be identified, namely F($\varphi: 0.75\pi \sim 1.5\pi$), N($\varphi: 1.75\pi \sim 2\pi \sim 0.5\pi$), Z($\varphi: 0.5\pi \sim 0.75\pi$) and S($\varphi: 1.5\pi \sim 1.75\pi$), consistent well with the previous investigation [12]. It is noteworthy that the correlation functions show the characterized values for these four phases as summarized in Table 1, which can be used to distinguish and monitor the phases.