Ground-state properties for bilayer Kitaev model: dimer expansion study

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Abstract We study ground state properties in the bilayer Kitaev model by means of the dimer expansion. The existence of parity symmetries in the system reduces the computational cost significantly. This allows us to expand the ground state energy and interlayer spin-spin correlation up to 30th order in the interdimer Kitaev coupling. The numerical calculations clarify that the dimer singlet state is indeed realized in the wide parameter region.

1 Introduction

Nonmagnetic states and the quantum phase transition have attracted much interest in frustrated quantum spin systems. One of the interesting examples is the two-dimensional orthogonal-dimer system [1,2], where nonmagnetic dimer and plaquette states compete with the antiferromagnetically ordered state [3]. Recently, the pressure-induced phase transition between the nonmagnetic states [4,5,6] has been observed in the candidate compound SrCu$_2$(BO$_3$)$_2$ [7], which stimulates theoretical investigations on the competition between nonmagnetic states [3,8]. Another interesting nonmagnetic state is the quantum spin liquid state in the Kitaev model [9], where spin degrees of freedom are decoupled into itinerant Majorana fermions and $Z_2$ fluxes [9,10,11,12,13]. Two energy scales for distinct degrees of freedom yield interesting finite temperature properties such as double peak structure in the specific heat, spin dynamics, and thermal Hall effect at low temperatures [14,15,16,17,18,19,20]. In our previous paper [21], we have considered two Kitaev models connected by the Heisenberg exchange couplings, which is one of simple models to discuss the effect of the interlayer coupling. Then, numerical calculations have suggested that the interlayer coupling induces the first order quantum phase
transition to a nonmagnetic dimer state. Here, we demonstrate the detailed analysis for the dimer expansion to clarify how stable the dimer singlet state is against the quantum spin liquid state.

In this work, we study the bilayer Kitaev model by means of the dimer expansion method, which is an approach from the state composed of interlayer dimer singlets, and discuss the stability of the dimer singlet state in the system. First, we explain the first order inhomogeneous differential method [22], where physical quantities are deduced from the series coefficients obtained from the dimer expansion. Then, we clarify that the dimer singlet state is indeed realized in the wide parameter region.

The paper is organized as follows. In §2, we introduce the model Hamiltonian on the bilayer Kitaev model. Then, we show the numerical results obtained by the dimer expansion and study the stability of the dimer singlet state. A summary is provided in the last section.

2 Model and Results

We consider the bilayer Kitaev model with the interlayer coupling, which should be given by the following Hamiltonian as, [see Fig. 1]:

$$\mathcal{H} = -J_K \sum_{\langle ij \rangle, \alpha, n} S_{i,n}^{\alpha} S_{j,n}^{\alpha} + J_H \sum_i S_{i,1} \cdot S_{i,2},$$  \hspace{1cm} (1)

where $S_{i,n}^{\alpha}$ ($\alpha = x, y, z$) is the $S = 1/2$ operator at site $i$ of the $n(=1, 2)$th layer, $J_K(>0)$ is the ferromagnetic Kitaev coupling in each layer, and $J_H(>0)$ is the antiferromagnetic Heisenberg coupling between two layers. In each layer, the anisotropy of the Ising-type interactions depend on the nearest neighbor bonds in the honeycomb lattice (see Fig. 1). When $J_H = 0$, the system is reduced to two single-layer Kitaev models, where the quantum spin liquid ground state is realized with gapless excitations [9]. On the other hand, in the case $J_K = 0$, the ground state is the direct product of interlayer dimer singlets with the spin gap. These two states have a difference in character, which should lead to the quantum phase transition between the two limits.

To clarify the stability of the dimer singlet state, we employ the dimer expansion technique [23,24,25]. Since this method combines the conventional perturbation theory with the cluster expansion, it has an advantage to deal with the frustrated spin system in higher dimensions, where the reliable results are hard to be obtained by quantum Monte Carlo simulations. In fact, using the dimer expansion, quantum phase transitions have been discussed in the frustrated spin systems such as the $J_1 - J_2$ [26], orthogonal-dimer [3,8,27], and Kitaev-Heisenberg models [28].

First, we divide the original Hamiltonian given by Eq. (1) into two parts. Since we start with the singlet state with strong $J_H$, the second term of Eq. (1)
Fig. 1  (Color online) Bilayer Kitaev model. Green, blue, and red lines represent the Ising interaction in the x, y, and z direction, and black lines the Heisenberg interaction.

Table 1  Series coefficients for the dimer expansion of the ground state energy $E_g/N = \sum a_i (J_K/J_H)^i$ and interlayer spin-spin correlation $\langle \mathbf{S}_1 \cdot \mathbf{S}_2 \rangle = \sum b_i (J_K/J_H)^i$ in the bilayer Kitaev model.

| $i$  | $a_i$       | $b_i$       | $i$  | $a_i$       | $b_i$       |
|------|-------------|-------------|------|-------------|-------------|
| 0    | -0.75       | -0.75       | 16   | 0.0725060850909 | -1.08759127636 |
| 2    | -0.1875     | -0.1875     | 18   | -0.09600123295502 | 1.63202096015  |
| 4    | 0.05859375  | -0.17578125 | 20   | 0.13044349648  | -2.47842643312 |
| 6    | -0.041015625 | 0.205078125 | 22   | -0.180983589717 | 3.80065538406  |
| 8    | 0.0376968383789 | -0.263877868652 | 24   | 0.255464209649  | -5.87567682193  |
| 10   | -0.0399161577225 | 0.359245419502 | 26   | -0.365835854119 | 9.14589635297  |
| 12   | 0.0461324302273 | -0.5074567325 | 28   | 0.530360009428  | -14.3197202546  |
| 14   | -0.0565949525058 | 0.735734382576 | 30   | -0.777038313098 | 22.5341110798  |

is considered as the unperturbed Hamiltonian $\mathcal{H}_0$, which is an assembly of interlayer singlet-dimer formed by the coupling $J_H$ [29,30]. In this bilayer Kitaev model, we use the following local basis sets given as

$$|s\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\downarrow_2\rangle - |\downarrow_1\uparrow_2\rangle), \quad |x\rangle = -\frac{1}{\sqrt{2}} (|\uparrow_1\uparrow_2\rangle - |\downarrow_1\downarrow_2\rangle), \quad (2)$$

$$|y\rangle = \frac{i}{\sqrt{2}} (|\uparrow_1\downarrow_2\rangle + |\downarrow_1\uparrow_2\rangle), \quad |z\rangle = \frac{1}{\sqrt{2}} (|\uparrow_1\downarrow_2\rangle + |\downarrow_1\uparrow_2\rangle), \quad (3)$$

where $|s\rangle$ is the singlet state and $|\alpha\rangle$ ($\alpha = x, y, z$) is the triplet state. Then, the corresponding eigenenergies for the local Hamiltonian $J_H \mathbf{S}_1 \cdot \mathbf{S}_2$ are $E = -3J_H/4$ and $J_H/4$, respectively. The interactions among independent dimers are taken into account by series expansions in the perturbed Hamiltonian $\mathcal{H}_1(= \mathcal{H} - \mathcal{H}_0)$. We wish to note that there exist global parity symmetries in the number of singlet and triplet states in this basis set [21]. Therefore, when
a certain cluster is concerned in the framework of the cluster expansion, the net states are restricted in the subspace with even number of triplet states for each component $\alpha$, which significantly reduce computation costs.

By performing the perturbation expansion for 787,894 graphs, we obtain the series coefficients for the ground state energy $E_g = \langle H \rangle$ and spin-spin correlations $C_s = \langle S_1 \cdot S_2 \rangle$ up to the 30th order in $J_K/J_H$. The results are explicitly shown in Table 1. We find that the series coefficients appear only in the even orders in $J_K/J_H$ and are alternating. Therefore, the extrapolations are necessary to deduce physical quantities in the large $J_K/J_H$ region.

Padé approximation is one of the powerful methods, where the function is approximated by the fractional of polynomials [22]. This method can access the intermediate region with $J_K/J_H \sim 1$, but we could not access the vicinity of the quantum phase transition point ($J_K/J_H \sim 17$) [21]. In this study, we make use of the extended method: the first-order inhomogeneous differential method [22]. In the method, the function $y(x)$ is numerically evaluated by the following differential equation as

$$xP_n(x)y'(x) + Q_n(x)y(x) = R_L(x),$$

(4)

where $P_n(x), Q_n(x)$, and $R_n(x)$ are the $n$th order polynomials of $x$. Since our obtained series has finite coefficients in even orders, we apply the method to $y(x) = q(x^2)$, where $x = J_K/J_H$ and $q = E_g, C_S$. Figure 2 shows the ground state energy and spin correlations deduced by the first-order inhomogeneous differential method, which is specified by $[N_0, N_1, L]$. The extrapolated values show good agreement with the results obtained by the exact diagonalization with $N = 24$ sites not only in the region of $J_K \sim 0$ but also $J_H/(J_H + J_K) > 0.15$, as shown in Fig. 2. Therefore, we can say that the dimer singlet state is indeed realized in the region. On the other hand, when $J_H/(J_H + J_K) \rightarrow 0.1$, we find pathological singularities in some curves, which sometimes occur in Padé and related methods. Although this makes it hard to deduce the physical quantities quantitatively in the region $J_H/(J_H + J_K) < 0.15$, one can expect that both quantities are smoothly changed. This is in contrast to the ED results for spin-spin correlations, where a rapid change appears around $J_H/(J_H + J_K) \sim 0.05$. This implies that the dimer expansion does not describe the ground state with $J_H/(J_H + J_K) < 0.05$, which suggests the existence of the first-order quantum phase transition between the dimer and quantum spin liquid states.

3 Summary

We have investigated ground state properties in the bilayer Kitaev model by means of the dimer expansion. By deducing the ground state energy and spin correlation between layers, we have confirmed that the dimer singlet state is indeed realized in the wide parameter region. The detail of the dimer expansion has been addressed.
Fig. 2 (Color online) Ground state energy and spin correlations in the bilayer Kitaev model. Symbols are the results obtained by the exact diagonalization with \( N = 24 \) sites [21]. Several lines with \([N_0, N_1, L]\) are obtained by the first-order inhomogeneous differential methods.

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