Magnetic properties of the $S = 1$ Kitaev model with anisotropic interactions

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We investigate magnetic properties in the $S = 1$ Kitaev model in the anisotropic limit. Performing the fourth-order perturbation expansion with respect to the $x$-bonds, $y$-bonds, and magnetic field, we derive the effective Hamiltonian, where the low-energy physics should be described by the free spins with an effective magnetic field. Making use of the exact diagonalization method for small clusters, we discuss ground-state properties in the system complementary.

1. Introduction

Recently, the Kitaev model [1] and its related models have attracted much interest since the possibility of the direction-dependent Ising interactions has been proposed in the realistic materials [2]. One of the important issues in this field is the ground-state property of Kitaev models whose the spin is generalized to an arbitrary $S$ [3–7]. In our previous paper [8], we have focused on the spin-$S$ Kitaev model in the anisotropic limit to clarify that the effective Hamiltonian depends on the magnitude of spins. When the spin is a half integer, the system is described by the toric code Hamiltonian and the topological nature of the ground state has been discussed in detail. On the other hand, in an integer-spin case, the effective Hamiltonian is equivalent to a free spin model under a uniform magnetic field, where quantum fluctuations are quenched. In contrast to the former case, ground-state properties in the spin-integer model are little understood. In particular, it is desired to discuss the effect of the magnetic field in the system.

In this paper, we study the $S = 1$ Kitaev model under the uniform magnetic field as a simplest model with integer spins and discuss ground-state properties by means of the perturbation theory and exact diagonalization (ED).

2. Model and Results

We consider the $S = 1$ Kitaev model under an external magnetic field, which is given as,

$$
\mathcal{H} = -J_x \sum_{\langle i,j \rangle_x} S_i^x S_j^x - J_y \sum_{\langle i,j \rangle_y} S_i^y S_j^y - J_z \sum_{\langle i,j \rangle_z} S_i^z S_j^z - h \cdot \sum_i S_i,
$$

(1)

where $S_i^\alpha$ is the $\alpha(= x, y, z)$ component of an $S = 1$ operator at the $i$th site. $J_\alpha$ is the exchange constant on the $\alpha(= x, y, z)$ bonds connecting the nearest-neighbor sites $\langle i, j \rangle_\alpha$. Here, we set $\mu B = 1$ and consider the magnetic field $h$ given by $h = h(\cos \varphi, \sin \varphi, 0)$. The model Hamiltonian is schematically shown in Fig. 1. It is known that, when no magnetic field is applied, a local $Z_2$ symmetry in the generalized Kitaev model plays an important role in realizing the quantum spin liquid state [3, 7]. On the other hand, when $h \neq 0$, there never exists such a symmetry and thereby it is unclear how stable the quantum spin liquid is against the magnetic field.
Now, we focus on the $S = 1$ Kitaev model in the anisotropic-exchange and weak-field limits $|J_x|, |J_y|, |h| \ll J_z$. In the case of $J_x = J_y = 0$ and $h = 0$, two adjacent spins on the $z$-bond $\langle i, j \rangle_z$ should be fully polarized as $|+1 \rangle_i |+1 \rangle_j$ or $|-1 \rangle_i |-1 \rangle_j$, where $|m\rangle_i$ is the eigenstate of $S^z_i$ with the eigenvalue $m(= -1, 0, 1)$ at the $i$th site. Therefore, it is convenient to introduce the pseudospin operator $\tilde{\sigma}_r$ on each $z$-bond $r$ so that $\tilde{\sigma}^z_r |\tilde{\sigma}^z_r\rangle_r = |\tilde{\sigma}^z_r\rangle_r$ with

$$ |	ilde{\uparrow}\rangle_r = |+1\rangle_i |+1\rangle_j, $$

$$ |	ilde{\downarrow}\rangle_r = |-1\rangle_i |-1\rangle_j, $$

where $\tilde{\sigma}$ takes +1 (\tilde{\uparrow}) or -1 (\tilde{\downarrow}). Now, we introduce $J_x$, $J_y$, and $h$ as perturbations to derive the effective Hamiltonian for low-energy states. Each perturbation includes $x$- or $y$-component of the spin operator, leading to the increment or decrement of local spin quantum number $m$ by 1. Therefore, the effective Hamiltonian appears from, at least, fourth-order perturbation. The perturbation processes should be represented by the exchange couplings connected to two pseudospins on the $x$ ($y$) bonds and magnetic field, which are schematically shown as the red (blue) lines and circles around a certain site in Fig. 2. By taking into account the corresponding contributions, we derive the effective Hamiltonian, as

$$ \mathcal{H}_{\text{eff}} = -h_{\text{eff}} \cdot \sum_r \tilde{\sigma}_r, $$

$$ h_{\text{eff},x} = \frac{7(J_x^2 - J_y^2)^2}{192J_z^3} + \frac{13(J_x^2 - J_y^2)h^2}{32J_z^3} \cos 2\varphi + \frac{5h^4}{4J_z^3} \cos 4\varphi, $$

$$ h_{\text{eff},y} = \frac{13(J_x^2 - J_y^2)h^2}{32J_z^3} \sin 2\varphi + \frac{5h^4}{4J_z^3} \sin 4\varphi, $$

$$ h_{\text{eff},z} = 0. $$

It is found that the effective Hamiltonian can be regarded as the free spin model with the effective magnetic field in the $x$ -- $y$ plane. Note that this effective field $h_{\text{eff}}$ is not directly related to the original magnetic field since it depends on not only $h$ but also the magnitudes of $J_x$ and $J_y$. Then, the ground state for the effective Hamiltonian is given by the direct product of the pseudospin state, as

$$ |g\rangle = \bigotimes_r \frac{1}{\sqrt{2}} \left[ |h_{\text{eff}}|(|\tilde{\uparrow}\rangle_r + |\tilde{\downarrow}\rangle_r) \right]. $$
In the system, the first excited energy is given by \(2|\hbar_{\text{eff}}|\) and a unique ground state is realized as far as the effective field is finite. By contrast, when \(\hbar_{\text{eff}} = 0\), the energy scale characteristic of this effective Hamiltonian vanishes. In the case, a higher order perturbation process should lift the macroscopic degeneracy in the low-energy states. Therefore, it is necessary to clarify how stable the ground state Eq. (8) is in the \(S = 1\) Kitaev model. In the following, we discuss the magnetic properties in the anisotropic \(S = 1\) Kitaev model.

First, we consider the \(S = 1\) Kitaev model without the external magnetic field [8]. When \(|J_x| \neq |J_y|\) and \(J_z \to \infty\), \(\hbar_{\text{eff},x} > 0\) and \(\hbar_{\text{eff},y} = 0\). Therefore the ground state satisfies \(\hat{\sigma}^y_i|g\rangle = |g\rangle\) for each \(z\)-bond. On the other hand, different behavior may appear in the symmetric case with \(|J_x| = |J_y|\) and/or away from the anisotropic limit \(J_z \to \infty\). To clarify how stable the ground state Eq. (8) is in the system with varying \(J_x\) and \(J_y\), we apply the ED method to the original model Eq. (1) on the 12-site and 18-site clusters shown in Fig. 1(b). Figure 3 shows the expectation value of magnetization \(\tilde{M}^x = \langle \hat{\sigma}^x \rangle = \langle S^x_i S^x_j - S^y_i S^y_j \rangle\) for the system with fixed \(J/J_z = 0.1, 0.2\), and 0.7, where \(J_x = J\cos \theta, J_y = J\sin \theta\). When \(\theta \neq \pi/4\) \((J_x \neq J_y)\), the expectation value is almost unity. In addition,

\[ \tilde{M}^x \]

\[ N=12, J/J_z=0.1 \]
\[ N=18, J/J_z=0.1 \]
\[ N=12, J/J_z=0.2 \]
\[ N=18, J/J_z=0.2 \]
\[ N=12, J/J_z=0.7 \]
\[ N=18, J/J_z=0.7 \]

Fig. 3. \(\theta\) dependence of the magnetization \(\tilde{M}^x\) in the ground state with \(J/J_z = 0.1, 0.2 \text{ and } 0.7\).
limit. These mean that the ground state of the system is well described by the effective Hamiltonian. We also find that, in the larger cluster, the region with $M^x \sim 1$ becomes larger, meaning that fourth-order Hamiltonian should capture a wide range of the parameter space in the thermodynamic limit. On the other hand, approaching $\theta \to \pi/4$ ($J_x \sim J_y$), the expectation value rapidly changes from the unity. As discussed above, the characteristic energy scale $\hbar$ vanishes at $\theta = \pi/4$, and macroscopic degeneracy is not lifted by fourth order perturbation in $J_x$ and $J_y$ shown in Figs. 2(a) and (b). In the case, other perturbation processes should be relevant. In fact, in the 12-site (18-site) cluster, fourth-order (sixth-order) perturbation process inherent in its periodic boundary lifts the ground-state degeneracy, resulting in $\tilde{M}^x \ll 0$. Therefore, we could not conclude the presence of such a drastic change in the magnetization $\tilde{M}_x$ around $\theta = \pi/4$ in the thermodynamic limit.

Next, we consider the effect of the external magnetic field in the system. In general, the effective Hamiltonian Eq. (4) well captures low-energy physics for the $S = 1$ Kitaev model with a large anisotropy. On the other hand, the ground state is not trivial when the characteristic energy scale vanishes, as discussed above. To examine the instability of the ground state, we solve $\hbar^\text{eff} = 0$. Besides the trivial solution with $|J_x| = |J_y|$ and $\hbar = 0$ discussed above, we find the other solution as,

$$h_0 = \left[\frac{7}{240} (J_x^2 - J_y^2)^2\right]^{1/4}$$

and

$$\varphi_0 = \frac{1}{2} \cos^{-1}\left(-\frac{13}{4} \sqrt{3} \frac{\sqrt{35}}{4} \right) \sim 0.450 \pi, 0.550 \pi \ (\text{mod} \ \pi).$$

Although this nontrivial solution is given in the anisotropic limit $J_z \to \infty$, it is unclear if this instability appears in the system with the intermediate coupling region. To examine how the characteristic energy scale depends on the magnitude and angle of the applied magnetic field, we numerically evaluate the lowest excitation gap $\Delta$ by means of the ED method for the 12-site and 18-site clusters. Figure 4 shows the comparison between $\Delta$ obtained by the ED method and that of the effective Hamiltonian, $2|\hbar^\text{eff}|$. When $J_x/J_z = 0.025$ and $J_y/J_z = 0.005$, we find little system-size dependence in the excitation gap. The angle dependence of the magnetic field is shown in Fig. 4(a), where the magnitude of the applied magnetic field is fixed as $\hbar = h_0$. Away from the $x$-axis (increasing $\varphi$), the excitation energy decreases and vanishes at $\varphi = \varphi_0$. In Fig. 4(b), we show the excitation gap in the system as a function of the magnitude of the magnetic field with a fixed $\varphi = \varphi_0$. It is clarified that the characteristic energy vanishes at $\hbar = h_0$. We also note that this energy is well reproduced by the fourth-order perturbation theory. These indicate that, in the $S = 1$ Kitaev model with the large anisotropy, there exists a certain magnetic field $h_0$, where the characteristic energy scale becomes too small. This instability is nontrivial, in contrast to the trivial solution $|J_x| = |J_y|$ and $\hbar = 0$. Therefore, it is interesting to observe this instability in the magnetization process experiments in the candidate materials [6].

### 3. Summary

We have studied low-energy properties of the $S = 1$ Kitaev model in the anisotropic limit, where one of the Kitaev couplings is large enough. By performing the perturbation expansion with respect to the other Kitaev couplings and magnetic field, we have obtained the fourth-order effective Hamiltonian, which is regarded as the free spin model under the effective magnetic field. Using the ED method with small clusters, we have discussed how stable the ground state for the effective model is in the $S = 1$ Kitaev model away from the anisotropic limit.
Fig. 4. Excitation gap as a function of (a) $\varphi$ [(b) $h$] in the system with $J_x/J_z = 0.025$, $J_y/J_z = 0.005$ and $h = h_0(\varphi = \varphi_0)$. Open (Filled) circles represent the results obtained from the ED method for the 12-site (18-site) system. The results obtained by the fourth order perturbation are shown as solid lines.

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