Sequential quantum phase transitions in $J_1-J_2$ Heisenberg chains with integer spins ($S > 1$): Quantized Berry phase and valence-bond solids

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On the basis of the Berry-phase analysis, we study the ground state of the $J_1-J_2$ Heisenberg chain for $S = 2, 3, 4$. We find that the changes of the Berry phase occur $S$ times for spin-$S$ systems, indicating the sequential phase transitions. The sequential phase transitions are associated with the change of valence-bond configurations of the ground states. To demonstrate this numerically, we connect the $J_1$-$J_2$ Heisenberg Hamiltonian with the generalized Affleck-Kennedy-Lieb-Tasaki model, and show that the different phases are connected to the different valence-bond-solid states.

I. INTRODUCTION

Over the past few decades, quantum spin chains with integer spin quantum numbers have provided us of a fertile ground for seeking topological phenomena in many-body physics. The $S = 1$ Heisenberg model with the nearest-neighbor (NN) interaction is a representative example. Its ground state is unique, has a short-range spin correlation, and hosts a finite energy gap on top of it. This state, which is called Haldane state [1, 2], is nowadays regarded as a representative example of the symmetry-protected topological phase [3–6] (SPT phase) in many-body quantum systems. Clearly, this phase is not characterized by the Ginzburg-Landau-type local order parameters. Indeed, for the $S = 1$ Heisenberg model, the ground state is characterized by the hidden valence-bond solid (VBS) state as inferred from the related model introduced by Affleck, Kennedy, Lieb, and Tasaki (AKLT) whose exact ground state is the VBS state [7, 8]. To capture such hidden structures in SPT phases, one needs to employ either non-local order parameters [8–10] or so-called topological order parameters [11–18]. Also, in many cases, characteristic boundary states for the open systems, e.g. the free end spins with $S = 1/2$ for $S = 1$ Heisenberg model [19], are the hallmark of the SPT phase [20, 21].

The richness of the phases becomes even abundant when considering the models beyond the simple NN-Heisenberg models, such as introducing the bond alternation [22–24] and a biquadratic term [7, 8, 25, 26]. In the present work, we focus on the $J_1-J_2$ Heisenberg model, where the next-nearest-neighbor (NNN) interaction ($J_2$) is introduced in addition to the NN interaction ($J_1$), resulting in the frustration. In the literatures [27–34], it was found that, upon changing the ratio of $J_2$ to $J_1$, the first-order quantum phase transition occurs near $J_2/J_1 \sim 0.75$. This phase transition is thought to be associated with the change of the corresponding VBS states [30]. Recently, Chepiga et al. found the change of the $\mathbb{Z}_2$ Berry phase [16, 35] across the phase transition, which is compatible with the change of VBS patterns [33].

Motivated by these works, in the present paper, we investigate the ground state of the $J_1$-$J_2$ Heisenberg chain for higher-order integer spins, $S = 2, 3, 4$. The models (up to $S = 2$, including XY/XXZ models) were investigated in Refs. 36–38, and Ref. 36 indicates the existence of the phase transition for the $S = 2$ Heisenberg chain, through the analyses of the end spins for the open systems. Based on these results, the goal of our study is to characterize the phase transitions by means of the Berry-phase analysis. We have found sequential changes of the Berry phase, which occur $S$ times for the spin-$S$ $J_1$-$J_2$ model, indicating sequential topological phase transitions. We further associate these transitions with the change of the VBS pictures of the ground states. It was argued in Ref. 30 that the phase for $J_2 < J_2^c$ and $J_2 > J_2^c$ correspond to NN-VBS state and NNN-VBS state [see Fig. 5(a) and 5(b)], respectively, for $S = 1$. To verify this scenario and further generalize it to the higher spins, we consider the models in which the Heisenberg model is continuously connected to the generalized AKLT models with various connectivity of singlets, and see whether the ground states are adiabatically connected upon changing the parameter. We find that the different phases in the $J_1$-$J_2$ Heisenberg chain is connected to the different VBS states, and that the number of phases for higher $S$ coincides with number of the possible VBS patterns.

The rest of this paper is organized as follows. In Sec. II, we first introduce the $J_1$-$J_2$ antiferromagnetic Heisenberg chain, which is the main focus of this paper. We also describe our method, namely, the detection of the topological phase transitions by using $\mathbb{Z}_2$ Berry phase. The details of the numerics are also elucidated. The main results of this paper are shown in Sec. III. First, we present the results of the $\mathbb{Z}_2$ Berry phase for $S = 2, 3, 4$. We show that there appear sequential changes of $\mathbb{Z}_2$ Berry phase

\begin{figure}[h]
\centering
\includegraphics[width=0.3\textwidth]{fig1.png}
\caption{The $J_1$-$J_2$ Heisenberg chain. The red and green lines represent the bonds where the twist of the interaction is introduced for the results in Sec. III A and III B, respectively.}
\end{figure}
as a function of $J_2/J_1$. We then move on to the analysis of the Heisenberg chain and the generalized ALKT models with various connectivities of singlets. Finally, we present a summary of this paper in Sec. IV.

II. MODEL AND METHOD

A. $J_1$-$J_2$ Heisenberg chain

We consider the $J_1$-$J_2$ antiferromagnetic Heisenberg chain for $S = 1, 2, 3$ and 4. The Hamiltonian reads

$$H^{(S)}_H = \sum_{i=1}^{N} J_1 S_i \cdot S_{i+1} + J_2 S_i \cdot S_{i+2},$$

where $S_i$ is a spin operator at site $i$, and $N$ is the number of sites. The exchange parameters, $J_1$ and $J_2$, are set to be non-negative. Hereafter, unless otherwise noted, we set $J_1 = 1$, as a unit of energy. We impose a periodic boundary condition, as $S_{i+N} = S_i$. See Fig. 1 for the schematic picture of the model. We note that, throughout this paper, we consider the finite chains whose ground states are accessible by the exact diagonalization (see Sec. II C for details).

B. $\mathbb{Z}_2$ Berry phase

For the gapped quantum systems, the Berry phase [35] with respect to the twist angles of boundary conditions is enforced to be quantized when the Hamiltonian has some discrete symmetries. Indeed, it has been served as a powerful tool to capture the topological phases in various systems with finite system size [16, 33, 39–52].

For the quantum spin systems having the time-reversal symmetry, $\mathbb{Z}_2$ Berry phase serves as a topological order parameter [16]. The Berry phase is defined with respect to the twist angle, $\theta$, which modulates the Hamiltonian in the following manner. The twist at the bond $(i, j)$ with the angle $\theta \in [0, 2\pi]$ is introduced by replacing $S_i \cdot S_j$ in the Hamiltonian with $\frac{1}{2} (e^{i\theta} S_i^+ S_j^- - e^{-i\theta} S_i^- S_j^+) + S_i^z S_j^z$. We label the Hamiltonian with the twist as $H(\theta)$. Suppose that the ground state of $H(\theta)$, $\{|\Phi_0(\theta)\rangle\}$, remains unique upon varying $\theta$. Then, one can define the Berry connection,

$$A(\theta) = \langle \Phi_0(\theta) | \partial_\theta | \Phi_0(\theta) \rangle,$$

and the corresponding Berry phase

$$i\gamma = \int_0^{2\pi} d\theta A(\theta).$$

Note that $\gamma$ is quantized as $\gamma = 0, \pi \pmod{2\pi}$ due to the time-reversal symmetry. Namely, the twisted Hamiltonian satisfies $TH(\theta)T^{-1} = H(-\theta)$, which leads to $\gamma = -\gamma \pmod{2\pi}$. Roughly speaking, $\gamma = \pi(0)$ indicates that there exist odd (even) number of hidden spin singles in the twisted bond(s) [16, 33, 41]. Therefore, it is useful for seeking the corresponding VBS picture of the ground state.

C. Numerical calculation of $\mathbb{Z}_2$ Berry phase

We numerically calculate the ground state $|\Phi_0(\theta)\rangle$ by the exact diagonalization. To obtain $\gamma$, the integration in Eq. (3) is approximated by the summation, as

$$i\gamma \sim \sum_{n=0}^{N_m-1} \Delta\theta \langle \Phi_0(\theta_n) | \partial_\theta | \Phi_0(\theta_n) \rangle,$$

where $\Delta\theta = \frac{2\pi}{N_m}$ and $\theta_n = n\Delta\theta$; $N_m$ is the number of meshes in a space of $\theta$. To avoid the gauge-fixing problem, the summation can be further approximated as follows [16, 53]. First, we define a quantity $U_n = \langle \Phi_0(\theta_n) | \Phi_0(\theta_{n+1}) \rangle$, which can be approximated up to the $O(\Delta\theta)$ as $U_n = 1 + \Delta\theta \langle \Phi_0(\theta_n) | \partial_\theta | \Phi_0(\theta_n) \rangle + O(\Delta\theta^2)$. Next, we introduce a gauge-invariant quantity $\log \prod_{n=0}^{N_m-1} U_n$, which can be approximated as

$$\log \prod_{n=0}^{N_m-1} U_n = \sum_{n=0}^{N_m} \langle \Phi_0(\theta_n) | \partial_\theta | \Phi_0(\theta_n) \rangle + O(\Delta\theta^2),$$

and thus we obtain $i\gamma \sim \log \prod_{n=0}^{N_m} U_n$.

As for the choice of the twisted bonds, we use three-bond twist, represented by red arrows in Fig. 1 for the results in Sec. III A. This choice is the same as that in the previous work [33], which turned out to reduce the finite-size effect. On the other hand, for the results in Sec. III B, we employ the single-bond twist, represented by a green arrow in Fig. 1, for the simplicity of calculations. It should be noted that both of the choices of the twisted bonds contain odd number of NN bonds and even number of NNN bonds, so the corresponding Berry phases should be the same, except for deviations due to the finite-size effect.

III. RESULTS

A. Sequential change of $\mathbb{Z}_2$ Berry phase for $S > 1$

In this subsection, we discuss the $J_2$ dependence of $\mathbb{Z}_2$ Berry phase for various $S$. The result for $S = 1$ was already uncovered [33], so we focus on the case with higher $S$. In Fig. 2, we show the $\mathbb{Z}_2$ Berry phase as a function of $J_2$ for $S = 2, 3, 4$. The system sizes we have used are presented in the caption. We clearly see the changes of $\gamma$ from 0 to $\pi$ or from $\pi$ to 0 when changing $J_2$, which indicate the quantum phase transitions. Notice that the changes occur $S$ times for the spin-$S$ model. For instance, for $S = 2$, the Berry phase varies as $0 \rightarrow \pi \rightarrow 0$, upon increasing $J_2$. Henceforth, we label n-th transition point for spin-$S$ model as $J_2^{(S,n)}$ (see red arrows in Fig. 2).
We further find another sign of the phase transition, namely the “hidden gap closing” when the twist is introduced. For the untwisted $J_1$-$J_2$ model, the energy gap between the ground state and the first excited state does not close across the change of the Berry phase. This behavior was also observed for $S = 1$ in the density matrix renormalization group (DMRG) study [28]. Our finding is that, at the critical values of $J_2$, the energy gap closes for the twisted model with $\theta = \pi$; see Fig. 3 for the energy gap as a function of $\theta$ at $J_2(2, 1)$. Note that similar behavior is argued in Refs. 54 and 55 in the context of the field-theoretical analysis.

As we have emphasized, the results shown in Fig. 2 is for the finite size system, and determination of the critical points in the thermodynamic limit is hampered by the finite size effect, as pointed out for $S = 1$ [33]. As an example, we show the size dependence of $J_2$ for $S = 2$ in Fig. 4. Clearly, the convergence of $J_2$ is not obtained up to $N = 12$. Therefore, one needs to employ an alternative method to obtain the precise critical points in the thermodynamic limit.

Although the existence of the phase transitions is captured $\mathbb{Z}_2$ Berry phase, the physical pictures of the phases can not be identified directly, which we will elucidate in the next subsection.

**B. Connection to the generalized AKLT models**

To understand the origin of the quantum phase transitions, we continuously connect the $J_1$-$J_2$ Heisenberg model with the generalized AKLT models whose ground states are the VBS states, up to $S = 2$.

The possible VBS states for the $J_1$-$J_2$ model are listed in Fig. 5. For $S = 1$, there are only two possible VBS states. One has the spin singlets in the NN bonds [NN-VBS state; see Fig.5(a)], whereas the other in the NNN bonds [NNN-VBS state; see Fig.5(b)]. For $S = 2$, on the other hand, there is the other state in addition to the NN-VBS and NNN-VBS states, in which the singlets live in both NN bonds and NNN bonds [Fig.5(d)]. We refer to this state as intermediate(I)-VBS state. To obtain the de-
sirable AKLT models, one can follow the recipe to write down the Hamiltonian with respect to the projection operators that favor the corresponding VBS states \[56, 57\]. In what follows, we employ

\[
H^{(1),(i)}_{\text{AKLT}} = 2 \sum_{i=1}^{N} P^1_2 (i, i + 1) = \sum_{i=1}^{N} \left[ S_i \cdot S_{i+1} + \frac{1}{3} (S_i \cdot S_{i+1})^2 + \frac{2}{3} \right],
\]

and

\[
H^{(1),(ii)}_{\text{AKLT}} = 2 \sum_{i=1}^{N} P^2_2 (i, i + 2) = \sum_{i=1}^{N} \left[ S_i \cdot S_{i+2} + \frac{1}{3} (S_i \cdot S_{i+2})^2 + \frac{2}{3} \right],
\]

for \( S = 1 \); similarly,

\[
H^{(2),(i)}_{\text{AKLT}} = 10 \sum_{i=1}^{N} \sum_{\delta=1,2} \left( \frac{1}{3} P^2_3 (i, i + 1) + P^2_4 (i, i + 1) \right)
\]

\[
= \sum_{i=1}^{N} S_i \cdot S_{i+1} + \frac{2}{9} (S_i \cdot S_{i+1})^2 + \frac{1}{63} (S_i \cdot S_{i+1})^3 + \frac{10}{7},
\]

for \( S = 2 \); here \( P^p_q (i, j) \) is a projection operator for total spin \( J \) of the bond \((i, j)\). The VBS state is a zero energy state of the Hamiltonian since it does not have any projection for the subspace \( J > 2S - M \) where \( M \) is a number of the valence bonds \[56, 57\].

Then, consider the Hamiltonian with additional parameter \( \lambda \in [0, 1] \):

\[
H^{(S)}(\lambda, \theta) = \lambda H^{(S)}_H (\theta) + (1 - \lambda) H^{(S)}_{\text{AKLT}} (\theta).
\]

Here \( \eta = (i), (ii), (iii) \) for \( S = 1 \) and \( \eta = (i), (ii), (iii) \) for \( S = 2 \). Notice that the twist of the Hamiltonian is introduced both in \( H^{(S)}_H \) and \( H^{(S)}_{\text{AKLT}} \). The higher-order terms of \( S_i \cdot S_j \) is twisted as \((S_i \cdot S_j)^a \rightarrow [\frac{1}{2} (e^{i\theta} S_i^a S_j^a + e^{-i\theta} S_i^a S_j^a)]^a + \alpha \) being a positive integer.

We aim to see whether the ground states of \( H^{(S)}_H \) and

\[
H^{(2),(ii)}_{\text{AKLT}} = 28 \sum_{i=1}^{N} \sum_{\delta=1,2} P^2_4 (i, i + \delta)
\]

\[
= \sum_{i=1}^{N} \sum_{\delta=1,2} S_i \cdot S_{i+\delta} + \frac{7}{10} (S_i \cdot S_{i+\delta})^2 + \frac{7}{45} (S_i \cdot S_{i+\delta})^3 + \frac{1}{90} (S_i \cdot S_{i+\delta})^4,
\]

\[
J_2(1, 1)
\]

FIG. 6. (a)-(d) \( \lambda \) dependence of the energy gap at \( \theta = \pi \) and the Berry phase of the Hamiltonian of Eq. (10) for \( S = \pm 1 \). The parameters and the choices of \( \eta \) for (a) \( J_1 = 1, J_2 = 0 \) and \( \eta = (i) \), (b) \( J_1 = 0, J_2 = 1 \) and \( \eta = (i) \), (c) \( J_1 = 1, J_2 = 0 \) and \( \eta = (ii) \), and (d) \( J_1 = 0, J_2 = 1 \) and \( \eta = (ii) \). The system size is \( N = 12 \). The gap closing occurs at \( \lambda = 0.4565 \) for (b), and \( 0.5185 \) for (c). (e) Schematic phase diagram of the \( J_1-J_2 \) model for \( S = 1 \) with respect to the VBS picture. Shaded area represents \( \gamma = \pi \).

FIG. 5. The schematic figures of the VBS ground states of (a) \( H^{(1),(i)}_{\text{AKLT}} \), (b) \( H^{(1),(ii)}_{\text{AKLT}} \), (c) \( H^{(2),(i)}_{\text{AKLT}} \), (d) \( H^{(2),(ii)}_{\text{AKLT}} \), and (e) \( H^{(2),(ii)}_{\text{AKLT}} \). The dots, lines, and open circles represent the spin 1/2, the spin singlets, and the symmetrization, respectively.
that of $H_{\text{AKLT}}^{(S)}$ are connected by introducing the Hamiltonian of Eq. (10). To this end, we monitor the energy gap upon varying $(\lambda, \theta)$. We also compute $\lambda$ dependence of the $Z_2$ Berry phase.

Let us first look at the results for $S = 1$, shown in Fig. 6. Clearly, the Heisenberg model with $J_2 < J_2^{(1)}(1,1)$ is connected to $H_{\text{AKLT}}^{(1),(i)}$ without gap-closing nor a change of the Berry phase [Fig. 6(a)], whereas that with $J_2 > J_2^{(1)}(1,1)$ is connected to $H_{\text{AKLT}}^{(1),(ii)}$ [Fig. 6(d)]. This indicates that the ground state of the Heisenberg model with $J_2 < J_2^{(1)}(1,1)$ is in the same phase as the NN-[NN-] VBS state, which is consistent with the previous study [30]. Also, the corresponding of the VBS states are consistent with the Berry phase [33], because there are odd (even) number of the singlets in NN- (NNN)-VBS state on NN bonds. In contrast, if the Heisenberg model is connected with the incompatible AKLT model, e.g., the Heisenberg model with $J_2 < J_2^{(1)}(1,1)$ and $H_{\text{AKLT}}^{(1),(ii)}$, the gap-closing at $\theta = \pi$ occurs, associated with the change of the Berry phase [Fig. 6(b)]. These results clearly illustrate that the change of Berry phase in the $J_1$-$J_2$ Heisenberg model upon varying $J_2/J_1$ originates from the phase transition from NN-VBS state to NNN-VBS state.

Next, we move on to the results for $S = 2$, shown in Fig. 7. Again, the different phases for the Heisenberg model are connected to the different VBS states, as NN-VBS state for $J_2 < J_2^{(2)}(2,1)$, I-VBS state for $J_2^{(2)}(2,1) < J_2 < J_2^{(2)}(2,2)$, and NNN-VBS state $J_2 > J_2^{(2)}(2,2)$. The number of the singlets on the NN bonds vary as $2 \rightarrow 1 \rightarrow 0$ upon increasing $J_2$, which is consistent with the profile of the Berry phase, $0 \rightarrow \pi \rightarrow 0$, as shown in Fig. 2(a). This result indicates that the sequential phase transition for $S = 2$ also originate from the change of the corresponding VBS states.

Considering the results on $S = 1$ and $S = 2$, it is inferred that, for general integer $S$, the $S$-time phase transitions for spin-$S$ models coincide with $S$ patterns of possible VBS states. Namely, for $J_2 = 0$, $S$ singlets live in the NN bonds, and upon increasing $J_2$, the number of singlets in NN bonds decreases as $S \rightarrow S - 1, \cdots \rightarrow 0$ and consequently the number of singlets in the NNN bonds increases as $0 \rightarrow 1 \rightarrow \cdots \rightarrow S$.

IV. SUMMARY

To summarize, we have investigated the ground state of the $J_1$-$J_2$ Heisenberg models with higher integer spins, by calculating $Z_2$ Berry phase. We reveal that spin-$S$ model undergoes $S$-time phase transitions. We attribute the sequential phase transitions to the change of VBS patterns, and demonstrate it by analyzing the models in which the $J_1$-$J_2$ Heisenberg model is continuously connected to the generalized AKLT models. The resulting VBS pictures are indeed consistent with the $Z_2$ Berry phase with respect to the parity of the number of singlets living in the twisted bonds.

All the results presented in this paper are for the finite-size systems with small number of sites accessible with the exact diagonalization. The precise determination of the critical values in the thermodynamic limit is outside of the scope of the present paper, and will be an important future problem.

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FIG. 7. (a)-(i) λ dependence of the energy gap at θ = π and the Berry phase of the Hamiltonian of Eq. (10) for S = 2. The parameters and the choices of η are (a) $J_1 = 1, J_2 = 0$ and η = (i), (b) $J_1 = 1, J_2 = 0.942$ and η = (i), (c) $J_1 = 0, J_2 = 1$ and η = (i), (d) $J_1 = 1, J_2 = 0$ and η = (ii), (e) $J_1 = 1, J_2 = 0.942$ and η = (ii), (f) $J_1 = 0, J_2 = 1$ and η = (ii), (g) $J_1 = 1, J_2 = 0$ and η = (iii), (h) $J_1 = 1, J_2 = 0.942$ and η = (iii), and (i) $J_1 = 0, J_2 = 1$ and η = (iii). The gap closing occurs at $λ = 0.855$ for (b), and 0.279 and 0.679 for (c), 0.881 for (d), 0.865 for (f), 0.257 and 0.715 for (g), and 0.731 for (h). The system size is $N = 9$. (j) Schematic phase diagram of the $J_1$-$J_2$ model for $S = 2$ with respect to the VBS picture. Shaded area represents $γ = π$.

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