Haldane and dimer phases in a frustrated spin chain: an exact groundstate and associated topological phase transition

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Abstract

A Heisenberg spin-$s$ chain with alternating ferromagnetic (FM) ($-J_F^1 < 0$) and antiferromagnetic ($J_A^1 > 0$) nearest-neighbor (NN) interactions, exhibits the dimer and spin-2s Haldane phases in the limits $J_F^1/J_A^1 \to 0$ and $J_F^1/J_A^1 \to \infty$ respectively. These two phases are understood to be topologically equivalent. Induction of the frustration through the next NN FM interaction ($-J_F^2 < 0$) produces a very rich quantum phase diagram. With frustration, the whole phase diagram is divided into a FM and a nonmagnetic (NM) phase. For $s = 1/2$, the full NM phase is seen to be of Haldane–dimer type, but for $s > 1/2$, a spiral phase comes between the FM and the Haldane–dimer phases. The study of a suitably defined string-order parameter and spin-gap at the phase boundary indicates that the Haldane–dimer and spiral phases have different topological characters. We also find that, along the $J_F^2 = \frac{1}{2}J_A^1$ line in the NM phase, an NN dimer state is the exact groundstate, provided $J_A^1 > J_C = \kappa J_F^1$ where $\kappa \leq s + h$ for applied magnetic field $h$. Without magnetic field, the position of $J_C$ is on the FM–NM phase boundary when $s = 1/2$, but for $s > 1/2$, the location of $J_C$ is on the phase separation line between the Haldane–dimer and spiral phases.

Keywords: Heisenberg spin chain, topological phase transition, Haldane gap, density matrix renormalization group method

(Some figures may appear in colour only in the online journal)

1. Introduction

In condensed matter physics a phase of a system can be identified by defining a suitable order parameter. However, it was later found that the phases can not always be characterized by the broken symmetry approach prescribed by Landau; here different phases are distinguished according to their topological characters [1, 2]. There are many systems where topology plays a vital role in characterizing their phases [1, 2]. For example, the antiferromagnetic Heisenberg spin chain can have gapped or gapless groundstate depending on whether site spins are integer or half-integer, as was first conjectured by Haldane [3]. The change in the spectrum of these systems can be explained by the topological terms in the field theoretical description of the spin chain [1, 3, 4]. Later it was shown that the Haldane phase in the odd and even integer spin ($S$) belong to different topological classes; while odd-$S$ Haldane phase is topologically nontrivial and protected by symmetries, even-$S$ Haldane phase is not protected and can be adiabatically transformed to a trivial site-factorizable phase [5]. It is also worth noting here that, there are topological phase transitions where the symmetry breaking takes place simultaneously (e.g. [6]).

Frustrated spin chain models, like ‘$J_1$–$J_2$’ model, have been extensively studied and they exhibit zoo of exotic quantum phases [7–14]. In this paper we study a frustrated quantum spin chain model, called here AFAF model, which has

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become a playground for studying and understanding the intricacies of the Haldane phase and its associated gap [15–18]. The AFAF model has alternating ferromagnetic (FM) (−J1F < 0) and antiferromagnetic (J1A > 0) nearest-neighbor (NN) exchange interactions. In this model the neighboring spin−s objects—connected by FM interactions—couple to form an effective spin-2s the Haldane chain in the limit J1F/J1A → ∞ [15–19]. This particular model got more prominence after it was realized experimentally in some materials, e.g., [Cu(TIM)]CuCl2 [20], (CH3)2CHNH2CuCl3 [21], CuNb2O6 [22], and (CH3)2NH2CuCl2 [23].

The main insight gained from studying the s = 1/2 AFAF model is the topological equivalence of the s = 1/2 the NN dimer phase (in J1F/J1A → 0 limit) and the s = 1 Haldane gapped phase (in J1F/J1A → ∞ limit). Hida first showed that the Haldane gapped phase is adiabatically connected to the NN dimer state [15] by studying the string-order parameter suggested by den Nijs and Rommelse as function of J1F/J1A [24]. Kohmoto et al supported this result by showing that the model has broken Z2 × Z2 hidden symmetry in both the phases [25, 26].

In this paper we study the rich phase diagram of the AFAF spin model with frustration which is induced by the next nearest-neighbor (NNN) FM interaction (−J2F < 0). With the frustration, the phase diagram shows two main phases—FM and nonmagnetic (NM). For s = 1/2, the whole NM phase is seen to be of gapped Haldane–dimer (HD) type, but for s > 1/2, we also obtain a spiral phase. The study of appropriately defined string-order parameter and spin-gap at phase boundary show us that the HD and the spiral phases are topologically different. We also show here that, an NN dimer state is the exact groundstate of spin model along J1F = 1/2J1A line, provided J1A > JC = κJ1F where κ ≃ s + h for applied magnetic field h. While the position of JC is on the FM–NM boundary for s = 1/2, but for s > 1/2, it is seen to be on the phase separation line between the topologically distinct HD phase and spiral phases.

This paper is arranged as follows. In the next section (section 2), we explain our spin model. In section 3, we briefly discuss equivalence of dimer and Haldane phases for spin-s AFAF model. Next in section 4, we discuss the phase diagram of the frustrated AFAF model—the discussion includes an exact dimer groundstate and the corresponding string-order parameter, and a spiral phase for s > 1/2. In section 5, we discuss a phase transition line (for s > 1/2) which separates the HD phase from a topologically different spiral phase. We then conclude our paper in section 6.

2. Frustrated AFAF model

The following Hamiltonian describes the frustrated spin-s AFAF chain of size N:

$$H = -J_1^F \sum_{k=1}^{N/2} \vec{s}_{2k-1} \cdot \vec{s}_{2k} + J_1^A \sum_{k=1}^{N/2} \vec{s}_{2k} \cdot \vec{s}_{2k+1}$$

$$-J_2^F \sum_{l=1}^{N} \vec{s}_l \cdot \vec{s}_{l+2} - h \sum_{i=1}^{N} s_i^z,$$

(1)

with J1F, J1A, J2F > 0. Here s’s are site spin operators with spin value s, J1A (J2F) is the NN FM (antiferromagnetic) exchange constant and J2F is the FM NNN exchange constant. The external magnetic field (h > 0) is applied along the z-direction. To make sure that the system reduces to an open spin-2s Haldane chain of even number of sites in the limit J1F/J1A → ∞, we only consider here, unless mentioned otherwise, the chain geometry where the first and the last bonds are FM in nature, and N ≡ 0 (mod 4).

3. Equivalence of dimer and Haldane phases

In the limit J1F/J1A → 0, the groundstate of the Hamiltonian in equation (1) with J2F = h = 0 is a product of NN dimers (here a dimer is the singlet between two spin-s objects). On the other hand, the model shows a spin-2s Haldane phase in the limit J1F/J1A → ∞. For s = 1/2, the dimer and Haldane phases are known to be adiabatically connected and topologically equivalent [15, 25, 26]. But this equivalence result is expected to be valid even for s > 1/2. This can be understood in the following way. Since different topological states can be distinguished by their groundstate degeneracies [2, 27], we will now calculate this quantity in two opposite limits. We first note that, in the dimer limit (J1F/J1A → 0), there exist two free spin-s objects at the two edges of the chain (see figure 1(b)); this gives rise to the (2s + 1)-fold groundstate degeneracy. In the Haldane limit (J1F/J1A → ∞), we get a spin-2s open chain of length N/2. The groundstate of this Haldane chain is actually topologically equivalent to the valence bond solid (VBS) state. The VBS state for spin-2s system can be obtained in the following way: each site spin can be considered as symmetric combination of two spin-s objects [28]. Now singlets can be formed between two spin-s objects from two neighboring sites (see figure 1(c)). This leaves two free spin-s objects at the two edges of the chain [5, 29]. This shows that, in the Haldane limit too, the groundstate degeneracy will be (2s + 1)2. The same value of the groundstate degeneracy in two opposite limits indicates that, the dimer and Haldane phases are topologically equivalent for all s.

It may be mentioned here that, for the odd-spin Haldane phase, four-fold degeneracy is genuine (as long as the time-reversal symmetry is maintained) and the rest of the degeneracy can be lifted by perturbations. On the other hand, for the even-spin Haldane phase, full degeneracy is accidental and can

Figure 1. (a) Left side of spin-s AFAF chain, (b) the dimer limit (J1F/J1A → 0); two spin-s objects are free at the edges, (c) the Haldane limit (J1F/J1A → ∞): after formation of VBS state, there will be two free spin-s objects left at the edges.
be lifted by perturbations [5]. The preceding discussion is valid in both the cases in the sense that it only shows the equivalence of the Haldane phase and the dimer phase, irrespective of whether those phases are topological trivial or not.

4. Extended phase diagram with frustration

To better understand the behavior of the Haldane and dimer phases under the frustration, and to investigate other possible quantum phases, we now study the AFAF model with frustration induced by the NNN ferromagnetic interactions (−J_2 \neq 0). In this section, we first show that an NN dimer state is the exact groundstate of the Hamiltonian in equation (1) along a special line in the parameter space. Then we exactly calculate a suitably defined string-order parameter and show that how our spin system behaves differently for integer or half-integer spin s. In the next two sub-sections, we respectively discuss a spiral phase (s > 1/2) and a ferromagnetic phase that appear in the phase diagram for J_2^v > 0.

4.1. Exact ground state

We begin by showing that, when J_2^v = 1/2 (we set J_1^v = 1 as normalization), an NN dimer state is an exact eigenstate of the Hamiltonian in equation (1). This dimer state is then proved to be the exact groundstate when J_1^v is larger than a critical value. Along the special line J_2^v = 1/2 in the parameter space, we rewrite the Hamiltonian in the following form (assume periodic boundary condition (PMB)):

\[ H = J_1^v \sum_{k=1}^{N/2} \vec{s}_{2k} \cdot \vec{s}_{2k+1} - \frac{1}{2} \sum_{k=1}^{N/2} \vec{s}_{2k} \cdot (\vec{s}_{2k-2} + \vec{s}_{2k-1}) - \frac{1}{2} \sum_{k=1}^{N/2} (\vec{s}_{2k} + \vec{s}_{2k+1}). \]  

(2)

Let [i, j] be the singlet state between spins at sites i and j. We then have the following relations: \( \vec{s}_i \cdot \vec{s}_j [i, j] = -\frac{s}{2} (s + 1) [i, j], \vec{s}_i \cdot (\vec{s}_i + \vec{s}_j) [i, j] = 0 \) for all \( k \neq i, j \) and \( (\vec{s}_i^z + \vec{s}_j^z) [i, j] = 0 \). Using these relations, it is easy to verify that the state \( \psi = [2, 3][4, 5][6, 7] \cdots [N, 1] \) is an eigenstate of the Hamiltonian \( H \) with the eigen energy \( E_0 = -\frac{N}{2} s(s + 1) J_1^v \), i.e.,

\[ H \psi = -\frac{N}{2} s(s + 1) J_1^v \psi. \]  

(3)

Using the Rayleigh–Ritz variational principle, it is possible to prove that this \( \psi \) is a groundstate of the system when \( J_1^v \) is greater than a critical value \( \kappa = J_C \) with \( J_1^v = 1 \). In the following we show that \( \kappa \leq s + h \).

Suppose that the total Hamiltonian of a system is written as the sum of M terms, i.e., \( H = \sum_{i=1}^{M} H_i \). Using the Rayleigh–Ritz variational principle, it can be shown that if a state is simultaneously a groundstate of each \( H_i \)’s, then it will also be a groundstate of the total Hamiltonian. To use this theorem for our purpose, we decompose \( H \) in equation (2) as

\[ H_{2k} = \frac{1}{2} J_1^v \vec{s}_{2k-2} \cdot \vec{s}_{2k-1} - \frac{1}{2} \vec{s}_{2k} \cdot (\vec{s}_{2k-2} + \vec{s}_{2k-1}) - \frac{h}{2} (\vec{s}_{2k} + \vec{s}_{2k-1}) \]  

(4)

\[ H_{2k-1} = \frac{1}{2} J_1^v \vec{s}_{2k} \cdot \vec{s}_{2k+1} - \frac{1}{2} \vec{s}_{2k} \cdot (\vec{s}_{2k+2} + \vec{s}_{2k+1}) - \frac{h}{2} (\vec{s}_{2k} + \vec{s}_{2k+1}). \]  

(5)

Here each part, represented by either \( H_{2k} \) or \( H_{2k-1} \), corresponds to a block of three spins. All these block Hamiltonians are essentially equivalent and have the same eigenvalues. Let us denote the Hamiltonian for this three-spin block as \( H_s \); considering the first triangle, we have \( H_s = \frac{1}{4} J_1^v (\vec{s}_i \cdot \vec{s}_j - \frac{1}{2} \vec{s}_s) \cdot (\vec{s}_s + \vec{s}_s) - \frac{h}{2} (\vec{s}_s + \vec{s}_s) \). In an earlier work [19], it was shown by explicitly forming and diagonalizing \( H_s \) with \( h = 0 \) that, the NN dimer state \( \psi \) is the groundstate of \( H \) for \( J_1^v \geq 0.5 \) when \( s = 1/2 \) and for \( J_1^v \geq 1.0 \) when \( s = 1 \). Numerically \( \kappa \) value is found to be 0.5 and 0.9 respectively for \( s = 1/2 \) and \( s = 1 \). We now extend this result for general spin \( s \), in addition, this time we also consider the presence of (weak) magnetic field \( h \).

First we rewrite \( H_s \) in the following way:

\[ H_s = -\frac{1}{4} (\vec{s}_i + \vec{s}_j + \vec{s}_s)^2 + \frac{1}{4} J_1^v + 1 (\vec{s}_s + \vec{s}_s)^2 \]  

\[ - \frac{h}{2} (\vec{s}_s + \vec{s}_s) + \frac{1}{2} \left( 1 - J_1^v \right) s(s + 1). \]  

(6)

The first two terms in equation (6) compete with each other and determine the nature of the groundstate in spin block. For example, if \( J_1^v \to 0 \), all three spins will try to form maximum possible total spin \( 3s \) and minimize the energy of \( H_s \). On the other hand, if \( J_1^v \gg 0 \), there will be a singlet formation between second and third spins to minimize the value of the second term in the expression of \( H_s \). Therefore, in the large \( J_1^v \) limit and in the presence of a weak magnetic field, the lowest energy of a three-spin block would be \( E_s = -\frac{1}{2} s(s + 1) + \frac{1}{4} \left( 1 - J_1^v \right) s(s + 1) = -\frac{h}{2} s(s + 1) \). For \( s \) such singlet state of three-spin blocks, the total energy for the whole system would be \( -\frac{3}{4} J_1^v s(s + 1) \) which have the value same as the eigen energy of the NN dimer state \( \psi \) in equation (5).

Therefore, following the theorem stated earlier, \( \psi \) will be the groundstate of the total system in the large \( J_1^v \) limit.

Now we try to estimate the critical value of \( J_1^v \), denoted here by \( J_C \), above which \( \psi \) is guaranteed to be the groundstate. In the phase diagram figure 2, the corresponding point is marked by \( C \). and \( ED \) marks a line along which \( \psi \) is an exact groundstate. For the estimation of \( J_C \), we first note the following tendency of a spin block. Let us first start with a large value of \( J_1^v \). Then, a singlet will be formed to minimize energy by increasing the absolute value of the first term and lowering the value of
the second term (see equation (6)). At the transition point, the singlet between the second and the third site would break and a triplet would be formed. In addition, the three spins together will form a spin \((s + 1)\) to maximize the absolute value of the first term. Correspondingly, the energy of the spin block would be \(E_i = -\frac{1}{2}(s + 1)(s + 2) + \frac{1}{4}(J_h^0 + 1)(1 + 1) - \frac{1}{2}(1 + 1) + \frac{1}{2}(J_h^0)(s + 1) = \frac{1}{2}J_h^0(s + 1) + \frac{1}{2}(J_h^0 - s - h)\).

The NN dimer state \(\psi\) will be the groundstate of the Hamiltonian in equation (2) as long as \(E_i \leq E_i\), i.e., when \(J_h^0 \geq s + h\). This gives us the upper bound of the critical value \(\kappa\), above which \(\psi\) is guaranteed to be the groundstate; so we have \(\kappa \leq s + h\).

To understand the character the point \(C\), we note for \(s = 1/2\) that, this point lies in the FM–NM transition line. For \(s > 1/2\), this point lies inside the NM region and the spin gap \((\Delta_S = \text{singlet–triplet gap})\) at this point is found to be zero within our numerical accuracy (more details on the FM and NM phases are given later). The relevant results on the spin gap for \(s = 1\) and \(s = 3/2\) can be found in figures 3(a) and 4(b) respectively. As the gap is expected to be zero at point \(C\), we call this point a critical point.

It is interesting to note here that, the NN dimer state is the exact groundstate of the spin model in two different limits of the extended phase diagram—along the line \(J_h^0 = \frac{1}{4}\) with \(J_h^0 > J_C\), and when \(J_h^0 = 0\) with \(J_h^0/J_h^0 \rightarrow 0\). The study of the spin-gap, string-order parameter and the entanglement spectrum for \(s = 1/2\) and 1 indicates that the dimer phases in those two limits are adiabatically connected and one does not encounter a quantum phase transition while going from one exact dimer groundstate to the other [19]. We expect this to be true for all values of \(s\). The adiabatic connectivity explains the continuity of the upper part of the phase diagrams in figure 2.

4.2. The string-order for dimer state

The topological equivalence between the dimer and the Haldane phases, as discussed in section 3, allows us to gain more insight into the nature of the Haldane phase by studying the topological character of the exact NN dimer groundstate. Here we first analytically calculate the string-order parameter \((O_2)\) for the exact dimer state. For our AFAF spin model, the string-order parameter is defined as: \(O_2 = \lim_{\lambda \rightarrow \infty} O_{2\lambda}\), where

\[
O_{2\lambda} = -\langle (\hat{s}_{12} + \hat{s}_{21} - s_2) \exp(i\pi \theta_{21}) (\hat{s}_{12} + s_2) \rangle,
\]

with \(\theta_{21} = (\hat{s}_{21} + \hat{s}_{21} + \hat{s}_{12} + \hat{s}_{12})\). We define \(O_{2\lambda}\) in such a way that, both \((\hat{s}_{21} + \hat{s}_{21})\) and \((\hat{s}_{12} + \hat{s}_{12})\) form a spin-2s object in the Haldane limit \(J_h^0/J_h^0 \rightarrow \infty\). Soon we will find that this definition of \(O_2\) produces result which is consistent with the earlier result that the odd and even spin Haldane phases are topologically nontrivial and trivial respectively.
The singlet (dimer) state between two spin-$s$ objects is given by $|d\rangle = \sum_{m=-s}^{s} \frac{1}{\sqrt{2s+1}} |m, m\rangle$; here basis $|a, b\rangle$ denotes a state where $z$-component of the first (second) spin is $a$ ($b$). The dimer groundstate of the spin-$s$ system can now be written as: $|\psi\rangle = \Pi_{i=1}^{L} |d_{2k,2k+1}\rangle$, where $|d_{2k,2k+1}\rangle$ denotes the singlet state between sites $2k$ and $2k+1$. While evaluating $O_{kl}$, we will assume that $|k - l| > 1$. Since $(s_{2k}^z + s_{2k+1}^z)|d_{2k,2k+1}\rangle = \exp(\pi i \theta_{kl})|d_{2k,2k+1}\rangle$, it is evident that, $\exp(\pi i \theta_{kl}) = \exp(\pi i (s_{2k+1}^z + s_{2k-1}^z))$ for the dimer groundstate $|\psi\rangle$. We also note that, due to the special form of the groundstate, $(s_{2k-1}^z \exp(\pi i \theta_{kl}) s_{2k}^z) = (s_{2k}^z \exp(\pi i \theta_{kl}) ) s_{2k-1}^z = 0$. With this information, $O_{kl}$ can now be written in the following form: $O_{kl} = -L \times R$, where $L = \langle d_{2k,2k+1} \rangle s_{2k} \exp(\pi i s_{2k+1}^z) |d_{2k,2k+1}\rangle$ and $R = \langle d_{2l-2,2l-1} \rangle \exp(\pi i s_{2l-2}^z) |d_{2l-2,2l-1}\rangle$. We note that the values of $L$ and $R$ are the same, and equal to $\langle d_{2k} | d_{2k+1} \exp(\pi i s_{2k}^z) \rangle |d_{2k+1}\rangle$. Therefore we can write,

$$O_{kl} = -\left( \langle d_{2k} | d_{2k+1} \exp(\pi i s_{2k}^z) \rangle \right)^2 = -\frac{1}{(2s+1)^2} \left( \sum_{m=-s}^{s} m e^{i \theta m} \right)^2 = \frac{4}{(2s+1)^2} \left( \sum_{m=-s}^{s} m \sin(\pi m) \right)^2,$$

where $a = 1$ or $1/2$ depending on whether $s$ is integer or half-integer respectively. After doing some algebra, we find from equation (8) that, $O_{kl} = 0$ or $1/4$ when $s$ is integer or half-integer. This simply shows that, the value of $O_{kl}$ for the NN dimer state is 0 or 1/4 depending upon whether $s$ is integer or half-integer.

The odd spin Haldane phase is a symmetry protected topological or SPT phase [30], on the other hand, the even spin Haldane phase is a trivial phase [5]. Since the spin-2s Haldane phase is topologically equivalent to the dimer phase of spin-$s$ AFAF model, we infer from the above result that the string-order parameter, as defined in equation (7), accurately identifies for our spin model whether a phase has topological character or not. We therefore use this suitably defined string-order parameter (as well as the spin-gap) to study different topological phases and associated topological phase transitions for our spin model (see section 5).

### 4.3. Ferromagnetic phase

The extended phase diagram of the frustrated AFAF model, as shown in figure 2, consists of a FM region and NM region. The FM region in the diagram enlarges as the ferromagnetic NNN interaction ($J^{r}_l \geq J^{r}_C$) increases in strength. A classical analysis [19, 31], as well as a wave-saw analysis [19], finds that the phase boundary between them is determined by $J^{r}_C = \frac{J^{r}_1}{2(1-J^{r}_1)}$ (setting $J^{r}_1 = 1$). The numerical studies for small spin ($s = 1/2$ and 1) show good agreement with this result [19].

For $s > 1/2$ and for a given $J^{r}_l$, the system goes from FM to NM spiral phase with increasing $J^{r}_l$. This phase transition can be explained in terms of the broken symmetry approach of Landau, and for the AFAF model, this particular phase transition has been studied [19, 31].

### 4.4. Spiral phase for $s > 1/2$

We already discussed that, our system is in dimer phase along $J^{r}_l = 1/2$ line as long as $J^{r}_l > J^{r}_C$. To know the nature of the phase for $J^{r}_l < J^{r}_C$, we do the structure factor analysis across the point $C$ for both $s = 1$ and $3/2$. We calculate the structure factor, $S(q)$, in the following way: $S(q) = \frac{1}{N} \sum_{m} s_{m}^\ast s_{m} \exp(-iqr_{m})$, where $<s_{m}^\ast s_{m}>$ is the correlation between the $z$-components of spins at sites $l$ and $m$, and $r_{m}$ is the distance between two sites ($r_{m} = m - l$). Here $N$ is the total number of spins in the system; for calculation of $S(q)$, we consider here an open chain with $\frac{N}{2}$th site as the reference. By convention the range of the wave vector is taken as: $0 < q < 2\pi$. The value corresponding to the maximum of $S(q)$ gives us the information about the ‘spin orientation’ in a particular quantum phase [for us $S(q)$ is always positive]. We see from figure 5 that, for both $s = 1$ and $3/2$, $q_{\text{max}}$ is close to but less than $\pi$ when $J^{r}_l < J^{r}_C$. $q_{\text{max}}$ is the $q$ value corresponding to the maximum of $S(q)$. This implies that we have a spiral phase below the point $C$ in the phase diagram figure 2. For $J^{r}_l > J^{r}_C$, $S(q)$ shows a broad peak at $q = \pi$—this finding is consistent with our result that in the said parameter regime we have a dimer phase which has short range correlation. After checking for some representative points in the phase diagram, we find that this spiral phase exists in the whole region between the ‘$ABCD$’ line and the FM phase. The said ‘$ABCD$’ line lies inside the NM phase and it separates the spiral phase from the HD phase. The character of the ‘$ABCD$’ line is discussed in the next section.

It may be mentioned here that this spiral phase does not appear for $s = 1/2$, for which the point $C$ falls in the FM–NM boundary. With increasing value of $s (>1/2)$, the location of the point $C$ is expected to go up (here we may remember that the calculated upper bound of $J^{r}_C$ is $s$ without magnetic field).
Our numerical results for $s = 1$ and $3/2$ support this expectation. So we conjecture here that this spiral phase exists for all $s > 1/2$. Next we will see that this particular spiral phase is topologically different than the HD phase.

5. Topological phase boundary

For $s > 1/2$, a spiral phase appears between the FM and the HD phases. The point $C$ lies on the phase boundary between the FM and HD phases (figure 2(b)). To understand the nature of the phase boundary, we study the string-order parameter and the spin-gap across the boundary.

As discussed earlier, the string-order parameter $O_3$, as defined in equation (7), accurately identifies for our spin model whether a phase has topological character or not. We inferred this from the fact that, $O_3$ is nonzero for the half-odd integer dimer state (which is topologically equivalent to an SPT phase) and $O_3$ is zero for the integer dimer state (which is equivalent to even spin trivial Haldane phase).

To characterize the nature of the phase boundary ['$ABCD$' line as appear in figure 2(b)], we first note that the system goes gapless at point $C$; this is verified for $s = 1$ and $3/2$ within our numerical accuracy. The relevant results on the spin gap for $s = 1$ and $s = 3/2$ can be found in figures 3(a) and 4(b) respectively.

We next study the string-order parameter ($O_3$) across the point $C$ along the $J_1 = 1/2$ line in the phase diagram. Above the point $C$, the NN dimer state is the groundstate, $O_3 = 0$ or $1/4$ depending of whether $s$ is an integer or half-integer (see earlier discussion). Below this point $O_3$ takes some other nonzero value (calculated numerically for $s = 1$ and $3/2$). We see a sudden change in $O_3$ at the point $C$. The relevant results for $s = 1$ and $3/2$ can be seen in figures 3(b) and 4(b) respectively. This sudden change in $O_3$ indicates that, the system goes through a first order topological phase transition at point $C$. But it may not be usual one, since the spin-gap at the point $C$ vanishes, which generally indicates a second order quantum phase transition. In fact, the transition point $C$ can also be viewed as the symmetry breaking phase transition point as it separates a dimer and a spiral phase. This type of concurrence of topological and symmetry breaking phase transitions is not new as mentioned in the introduction of this paper. It is also worth noting that, both for integer and half integer spin cases, the point $C$ appears to be a topological phase transition point although only for half integer case the dimer phase is an SPT phase. A more extensive study is needed to have better understanding on this issue.

A topological phase transition point can not be an isolated point inside the phase diagram, as otherwise a particular phase can be shown to have two different topological characters. We therefore expect, for our frustrated AFAF spin model, the point $C$ to lie on a topological phase transition line which spreads across the phase diagram. To confirm that the line ['$ABCD$' in figure 2(b)] is actually a topological phase transition line, we study $O_3$ across some representative points along the line. For example, when $J_1^F = 0.4$, we find that the change in $O_3$ across the line becomes sharper with the increasing system size [see inset of figure 3(b)]. This suggests that the ‘$ABCD$’ is a topological phase transition line which separates the HD phase from the spiral phase.

6. Concluding remarks

In this paper we study the topological aspect of AFAF model for general spins. In two opposite limits of $J_2^F/J_1^F$, this model gives two phases—the spin-$2s$ Haldane and dimer, where latter one results from singlet formation between two neighboring spin-$s$ objects. To have broader understanding of the physics of the model, we study it with frustration which is induced by the NNN FM interactions ($J_3^F > 0$). For the frustrated AFAF model, the NN dimer state is shown to be the exact groundstate provided $J_2^S \geq J_C$ and $J_2^S = 1/2$. We also show that the frustrated spin model for $s = 1/2$ and $s > 1/2$ behave differently: while in the first case the phase diagram consists of a FM and a NM (HD) phase, in the later case, the model additionally shows a NM gapped spiral phase which comes between the HD and FM phases.

The study of a suitably defined string-order parameter and spin-gap at the phase boundary indicate that the boundary separating the HD and spiral phases is a topological phase transition line both for integer and half-integer spins although only half-integer dimer phase has nontrivial topology. The spiral phase for both types of spins appears to have nontrivial topological order. Interestingly, our studies indicate that the phase boundary line can also be viewed as the second order symmetry breaking phase transition line. A more detailed study on the spin model is needed in future to gain better understanding on this issue.

The present work sheds some light upon the intricacies related to the Haldane physics and opens a new avenue to investigate the many body topological phases. The AFAF model has already been realized in many systems, and this work may excite the experimentalists to design new compounds and study topological phase transitions.

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Appendix. Numerical methods

We have used the density matrix renormalization group (DMRG) method, which is a powerful numerical technique for studying 1D and quasi-1D systems [32, 33]. In this technique the truncation of the irrelevant degrees of freedom is done systematically. For the calculations in this article, we employ PBC and for that we use a recently developed efficient DMRG algorithm for systems with PBC [34]. In this algorithm we start with a superblock that consists of eight sites: two sites in the left and the right block, and two new sites at both the ends of both the blocks. The left and right blocks increase by four sites
as two new sites are added at both the ends of each block. In this way we avoid the long bond between the old blocks. Here, we have kept up to \( m = 500 \) eigenvalues of the density matrix to keep the largest truncation error below \( 10^{-11} \).

The spin gap \( \Delta_S \) is defined as the difference between the singlet groundstate and the triplet first excited state:

\[
\Delta_S(N) = E_0(S^z = 1, N) - E_0(S^z = 0, N), \tag{A1}
\]

where \( E_0(S^z = 1, N) \) is the lowest energy in the total \( S^z = 1 \) sector i.e., the lowest triplet energy and \( E_0(S^z = 0, N) \) is the lowest energy in the total \( S^z = 0 \) sector i.e., singlet groundstate energy for a ring of \( N \) spins. Calculation of \( \Delta_S \) using DMRG is straightforward as our algorithm uses \( U(1) \) symmetry to conserve the total \( S^z \).

The string order parameter, \( O_3 \), used in this work is defined in equation (7). In our calculations, we consider FM interaction \( J' \) between the new sites at the both ends of the left or right block. The left block is numbered from \( 2k + 1 \) to \( 2l \) whereas, \( 2k - 1, 2k, 2l - 1, 2l \) are the new sites.

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