Reentrance of the topological phase in a spin-1 frustrated Heisenberg chain

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(Received 17 May 2019; revised manuscript received 8 December 2019; published 29 January 2020)

For the Haldane phase, the magnetic field usually tends to drive the system into a topologically trivial phase. Here we report a novel reentrance of the Haldane phase at zero temperature in the spin-1 antiferromagnetic Heisenberg model on a sawtooth chain. A partial Haldane phase is induced by the magnetic field, which is the combination of the Haldane state in one sublattice and a ferromagnetically ordered state in the other sublattice. Such a partial Haldane phase should be protected by the bond centered inversion symmetry, and is a result of the zero-temperature entropy due to quantum fluctuations and geometrical frustration.

DOI: 10.1103/PhysRevB.101.045133

I. INTRODUCTION

Frustration incorporating with strong correlations usually leads to exotic quantum phenomena. A typical example in statistical physics is the reentrant phenomena, where a sequence of phase transitions, such as A-B-A-B by lowering temperature may happen, where A and B denote ordered and disordered phases, respectively. Taking the Ising model on a kagomé lattice with nearest and next-nearest neighboring interactions as an example, one may find that upon lowering temperature, the system passes through four phases: a paramagnetic phase, a magnetically ordered phase, a reentrant paramagnetic phase, and a ferromagnetic phase [1]. Such a reentrant phenomenon was experimentally confirmed [2] and theoretically investigated with different approaches [1,3–8]. In the past decades, systematic investigations on the partially disordered phase in both classical and quantum systems at finite temperatures were performed theoretically [1,4,5,9–15] and experimentally [16–21]. It has been widely recognized that the partially disordered phase is driven by the thermal entropy, in which the disordered part behaves like a "perfect" paramagnet. The reentrant phenomena can be viewed as the order-by-disorder effect [22], which is driven by thermal fluctuations and entropy.

Recently, interests on the reentrant phenomena were renewed. The order-by-disorder effects were investigated theoretically [23–26] and experimentally [27,28]. For the spin-$1/2$ Heisenberg antiferromagnet on the $\sqrt{3}\times\sqrt{3}$-disordered triangular lattice [26], a partially disordered ground state in the weakly frustrated regime was reported. The spins on the honeycomb sublattice form a 180° Néel order, and spins at the hexagon center sites are in a disordered state. This work is aimed at explaining the spin-liquid behaviors of $LiZn_2Mo_3O_8$ [29], and shows that a partially disordered phase can be the ground state of a simple quantum isotropic Heisenberg antiferromagnet. Comparing with the classical systems, the disordered subsystem is a short range ferromagnetically correlated state instead of a paramagnet, and the mechanism is owning to the zero-point quantum fluctuations instead of the thermal ones. Furthermore, previous works show that the order-by-disorder effects are observed not just on the frustrated magnets [23] but also in cold-atom platforms [25]. The quantum fluctuations might be induced by, for instance, the spin-orbit couplings [24,25].

In this paper we study the spin-1 Heisenberg model on the sawtooth chain (Fig. 1) by a density matrix renormalization group [30]. The sawtooth chain is an important one-dimensional (1D) structure that widely exists in natural materials (e.g., $Cu_2Cl(OH)_3$ [31]). The model Hamiltonian is given as

$$H = J_1\sum_i \mathbf{S}_i\cdot\mathbf{S}_{i+1} + J_2\sum_{\text{odd i}} \mathbf{S}_i\cdot\mathbf{S}_{i+2} - h_z\sum_i S_i^z, \tag{1}$$

where $J_1=\cos(\frac{\pi}{2}\theta)$, $J_2=\sin(\frac{\pi}{2}\theta)$ $(0\leqslant\theta\leqslant 1)$, and h_z is the magnetic field along the z direction. We report a reentrance of the Haldane phase in this model at zero temperature. The calculational details are given in the Supplemental Material [32]. We establish the θ-h_z phase diagram of the system (Fig. 2), where two topologically nontrivial phases (Haldane and partial Haldane phases) are found. In the partial Haldane phase, only one sublattice of the system is in the Haldane phase (sublattice A in Fig. 1), and sublattice B is in a topologically trivial phase. Particularly for $\theta\simeq 0.62$, a reentrance of the topological Haldane phase induced by the magnetic field h_z is revealed. The Haldane phase–trivial magnetic phase–partial Haldane phase transitions by increasing h_z are discovered. The partial Haldane phase appears by increasing the magnetic field. For $h_z=0$, the Haldane phase is protected by any one of the three symmetries, say the time reversal symmetry,

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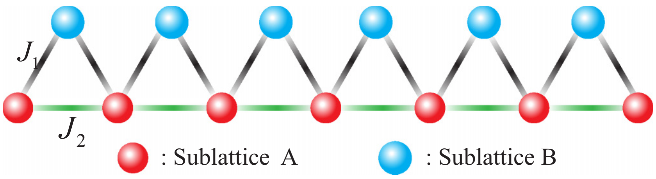

FIG. 1. Sawtooth chain lattice with two sublattices A and B. Two exchange interactions J_1 and J_2 are indicated by black and green lines, respectively.

D_2 symmetry, and bond centered inversion symmetry [33]. In the partial Haldane phase, although the time reversal symmetry of the whole system is broken by the external magnetic field, the bond centered inversion symmetry still exists. Therefore, the system reenters the Haldnae phase even in the magnetic fields that are larger than the Haldane gap. Our work extends the quantum reentrant phenomena at zero temperature from the conventional phases (e.g., [26]) to topological phases.

II. PHASE DIAGRAM

We establish the phase diagram in the θ-h_z plane as shown in Fig. 2. The phase boundaries are determined by several quantities including the uniform and staggered magnetizations of the sublattices, the local magnetic moments, and the entanglement entropy measured in the middle of the system. The phase diagram consists of seven quantum phases, including two gapless magnetic phases [up-up-up phase (UUU) and up-down-down (UDD) phase with the spins pointing down (up)

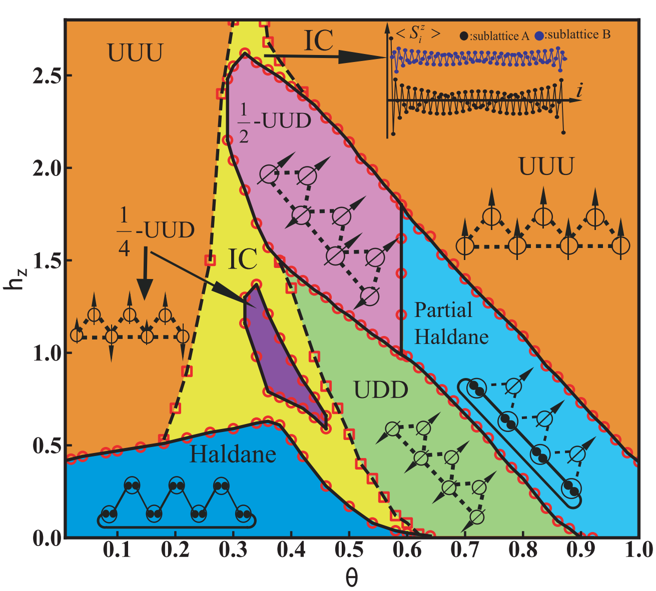

FIG. 2. The phase diagram in the θ-h_z plane obtained by our finite DMRG algorithm with a periodic boundary condition. The length of the sawtooth chain is $L = 160$ and the truncated dimensions is $\chi = 160$. There exists a phase crossover region, which is surrounded by a dashed line. There are two gapless magnetic ordered phases (UDD and UUU), and two gapped magnetic plateau phases ($\frac{1}{4}$-UUD and $\frac{1}{2}$-UUD). There appear two topological ordered phases, the Haldane phase and partial Haldane phase.

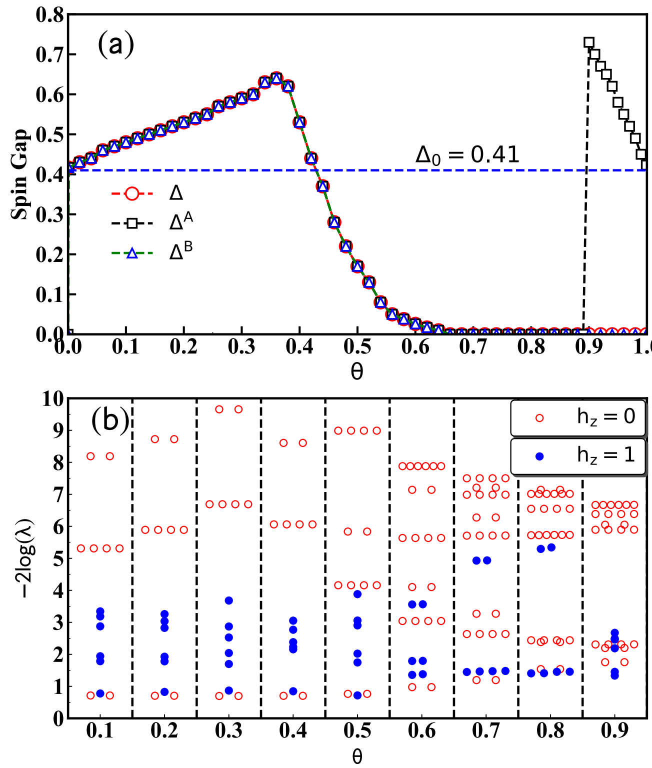

FIG. 3. (a) Spin gap Δ, Δ^A, Δ^B versus θ with $h_z = 0$. (b) Entanglement spectra versus θ, where the number of dots on each level indicates its degeneracy. The red circles and the blue dots represent the cases of $h_z = 0$ and $h_z = 1$, respectively.

on the sublattice A (B)], two gapped magnetic plateau phases [up-up-down phases on the $M = \frac{1}{4}$ plateau ($\frac{1}{4}$-UUD) and $M = \frac{1}{2}$ plateau ($\frac{1}{2}$-UUD)], an incommensurate crossover (IC) region, and two topological phases (Haldane phase and partial Haldane phase). The IC and UUU are connected by crossover (implied by dashed lines) with no singular behaviors [34].

Let us focus on the Haldane phase and partial Haldane phase. We first consider two limits $\theta = 0$ and $\theta = 1$. In the case of $\theta = 0$, we have $J_1 = 1$ and $J_2 = 0$, and the system becomes a standard spin-1 antiferromagnetic Heisenberg chain. The ground state in this case is the well-known Haldane phase (HP) [35,36] with a finite gap $\Delta_0 = 0.41J$ [30,37]. In the case of $\theta = 1$, we have $J_1 = 0$ and $J_2 = 1$, the system can be regarded as a Haldane chain in sublattice A, decoupled to the free spins in sublattice B.

Fruitful physics appear at $0 < \theta < 1$. Figure 3(a) shows $\Delta^{A(B)}$ and Δ that are the spin gaps of sublattices A (B), and that of the whole lattice. They are determined by the width of the zero plateau of the magnetizations $M^{A(B)} = \frac{2}{N}\sum_{i\in A(B)}\langle S_i^z\rangle$ and $M = (M^A + M^B)/2$, with N the total number of sites. For $\theta = 0$, all Δ and $\Delta^{A(B)}$ are close to $\Delta_0 = 0.41J$, which is the gap of the standard Haldane chain. By increasing θ, the spin gaps increase monotonously until $\theta \simeq 0.38$, where the gaps reach a maximum about $\Delta = \Delta^{A(B)} \simeq 0.62$. Afterwards, the spin gaps decrease rapidly and vanish at $\theta_{c1} \simeq 0.64$. For $\theta > \theta_{c1}$, the system enters a gapless region with $\Delta = \Delta^{A(B)} = 0$ until θ reaches $\theta_{c2} \simeq 0.9$. For $\theta_{c2} < \theta < 1$, Δ^B remains zero (thus $\Delta = 0$), but Δ^A jumps to a finite value, which indicates that sublattice A enters the Haldane phase. In this region, subsystem B is sensitive to the external field and can be polarized by a very small h_z, similar to a paramagnet. By increasing θ to $\theta = 1$, Δ^A approaches $\Delta^A = \Delta_0$, where the system becomes a Haldane chain decoupled with free spins.

Figure 3(b) demonstrates the entanglement spectra (ES) of the ground state. It has been suggested that ES can be used to characterize and classify exotic quantum states that are beyond the Landau symmetry-breaking paradigm [33,38–40]. In particular, the phase transition from the Haldane phase to a topological-trivial phase can be detected by the collapse of the even-fold degenerate structure of the ES [33,41]. Previous work proved that the Haldane phase is stable as long as an appropriate set of symmetries (time reversal symmetry, D_2 symmetry, or bond center inversion symmetry) are preserved [33,42,43]. In this sense, the Haldane phase can be separated from the topologically trivial phases, between which the gap closes at the phase boundary [33]. At relatively large magnetic fields, our sawtooth model reenters the Haldane phase that should be protected by the bond centered inversion symmetry. Note a spatial symmetry does not induce gapless edge modes.

It is possible that the terms like J_2 may destroy the Haldane phase as in, e.g., the spin-1 J_1-J_2 chain for $J_2 > 0.75$ [44,45]. In our system for $h_z = 0$, the ES [red hollow circles in Fig. 3(b)] versus θ shows that the even-fold degeneracy structure always appears in the whole range of $0 < \theta < 1$. It suggests that the J_2 terms do not break the symmetries that protect the topological phase, and the system remains in the Haldane phase in the whole range of θ.

At $\theta = \theta_{c2} \simeq 0.9$, where the gap of sublattice A is opened [black squares in Fig. 3(a)], we do not see any singularity from the entanglement entropy or energy. The system should be formed by a Haldane state in sublattice A, which contributes the twofold degeneracy, and the free spins in sublattice B. We speculate that $\theta = \theta_{c2}$ might be a topological phase transition point that separates two phases with different string orders [35,36]. See the Supplemental Material for details [32].

Figure 3(b) also shows the ES versus θ at $h_z = 1$ (blue solid circles). In accordance with the phase diagram, no double degeneracy of the ES is observed for $0 < \theta < 0.59$ and $0.83 < \theta < 1$. These regions are formed by several phases such as magnetic plateaus and incommensurate regions which possess no topological orders. For $0.59 < \theta < 0.83$, the system is in the partial Haldane phase, showing a fourfold degeneracy of the ES. Note that in the Haldane phase for $h_z = 0$ [see the red circles in Fig. 3(b)], the dominant two numbers of the ES is degenerate, and the next-dominant part shows fourfold degeneracy. One possible reason for the dominant fourfold degeneracy in the partial Haldane phase (say $h_z = 1$) is that the next-dominant part with fourfold degeneracy in the Haldane phase is shifted down to the part with twofold degeneracy. However, we cannot give more evidences to explain the fourfold degeneracy, and leave it as an open question.

Within the partial Haldane phase, the state is on a $M = \frac{1}{2}$ magnetic plateau. As shown in Figs. 2 and 3(a), the width of the 1/2 plateau gives exactly the spin gap of sublattice A. Note that the $\frac{1}{2}$-UUD also shows a 1/2 plateau,

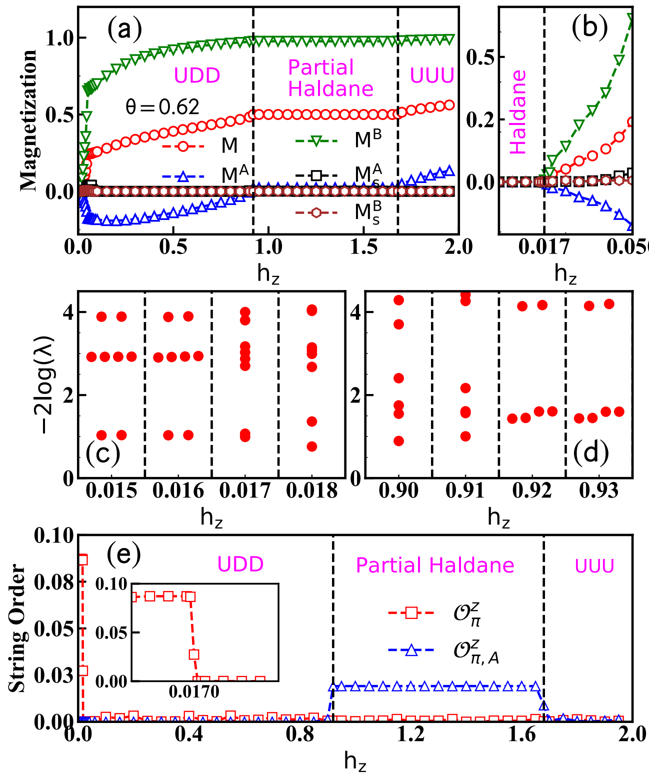

FIG. 4. Detailed description of M, M^A, M^B, M_s^A with fixed $\theta = 0.62$, where h_z is in the range of [0, 2] in (a). (b) The enlarged part of (a), where h_z is in the range of [0, 0.05]. The ES is illustrated in (c) and (d) in the vicinities of $h_z = 0.017$ and $h_z = 0.92$, respectively. (e) Two kinds of string orders O_π^z and O at $\theta = 0.62$. The inset shows the details of O_π^z in the range of $0 < h_z < 0.035$. At $h_z = 0.017$, O_π^z jump to zero, which is the transition point from Haldane phase to UDD magnetic ordered phase.

however, the magnetic order of sublattice A is completely different from the partial Haldane phase.

III. REENTRANCE OF TOPOLOGICAL PHASES

Normally, topological phases including Haldane phase will be suppressed by the magnetic field. For a gapped SPT phase, the magnetic field tends to close the energy gap and drives the system to a trivial magnetic phase. In our system we show that the partial Haldane phase that exhibits topological order will be induced by increasing the magnetic field. The Haldane–trivial phase–partial Haldane quantum phase transitions are observed. Figure 4 presents such a reentrant behavior by showing the magnetizations and ES at $\theta = 0.62$. For $h_z < h_{c1} \simeq 0.017$, all magnetizations are zero, and the ES shows twofold degeneracy [Figs. 4(b) and 4(c)]. The system is in the Haldane phase. For $h_z > h_{c1}$, the system is driven to UDD phase. This is a topologically trivial phase, where the spins shows long-range magnetic orders. The degeneracy of the ES is also lifted in this phase. By continuing increasing h_z to $h_z > h_{c2} \simeq 0.91$, the system is driven back to a topological phase (partial Haldane phase) with twofold degeneracy in the ES [Fig. 4(d)]. Until $h_z > h_{c3} \simeq 1.69$, the system enters a UUU phase.

At $\theta = 0.62$, the reentrance of the topological phase is further revealed by the string orders O^z_π and $O^z_{\pi,A}$, which are defined as

$$O^z_\pi(i,j) = \left\langle \hat{S}^z_i \exp\left(\sum_{k=i+1}^{j-1} i\pi \hat{S}^z_k\right) \hat{S}^z_j \right\rangle, \tag{2}$$

$$O^z_{\pi,A}(i,j) = \left\langle \hat{S}^z_i \exp\left(\sum_{k=i+1, i\in A}^{j-1, j\in A} i\pi \hat{S}^z_k\right) \hat{S}^z_j \right\rangle, \tag{3}$$

where $O^z_{\pi,A}$ is defined on sublattice A, and O^z_π is defined on the whole lattice. Note that O^z_π and $O^z_{\pi,A}$ are calculated in the middle of the chain by taking a sufficiently large distance ($|i-j| \simeq 140$). For $h_z < 0.017$, the system is in the Haldane phase with $O^z_\pi \simeq 0.095$ and $O^z_{\pi,A} \sim O(10^{-20})$. In the partial Haldane phase for $0.91 < h_z < 1.69$, we have $O^z_{\pi,A} \simeq 0.019$ and $O^z_\pi \sim O(10^{-4})$. Actually, string order is a very fragile order parameter; it decays when there exist small perturbations [46]. In some cases, the string orders might be absent even in the Haldane phase, thus the degeneracy of ES is considered as a more robust quantity to define the Haldane phase [33].

The reentrance of the topological phases can also be understood with the following intuitive picture. In the Haldane phase (including $h_z = 0$ and an arbitrary θ), all spins participate in the Haldane state, where each spin-1 is considered as a triplet formed by two effective spin-1/2's, and each two effective spin-1/2's from the two adjacent spin-1's form a singlet (valence bond). With a small but nonzero h_z, the system enters the UDD magnetic phase for $0.64 < \theta < 0.9$, where the spins in the two sublattices are towards different directions. Due to the geometrical frustration, sublattice B plays the role of a ferromagnetic background that provides an effective magnetic field (denoted as h_{inner}) to sublattice A with $h_{\text{inner}} \propto M^B$ (in the opposite direction to h_z). The spins in sublattice B are (nearly) polarized by a small h_z, inducing a large h_{inner}. Therefore, for a small h_z, sublattice A is actually in the field $h_{\text{effect}} = h_z - h_{\text{inner}}$, which is strong enough to close the Haldane gap ($\simeq 0.41J$). Thus, sublattice A cannot form a Haldane state for a small (but nonzero) h_z. This explains why this region is gapless, where h_{inner} instead of h_z is responsible to close the Haldane gap.

For $\theta = 0.64$ and $h_z > 0.97$, the spins in sublattice B are totally polarized, and h_z is strong enough to cancel with h_{inner}, so that the total effective field $h_{\text{effect}} = h_z - h_{\text{inner}}$ on sublattice A is beneath the Haldane gap. In this case, the spins in sublattice A form a Haldane state, and the whole system reenters the partial Haldane phase. This is similar to the standard Haldane phase in the spin-1 chain with $h_z < \Delta_0$. Thus we believe that the inversion symmetry protecting the Haldane and partial Haldane phases should be the same. By further increasing h_z, the magnetic field is sufficiently large to drive the system out of the partial Haldane phase and polarizes all spins in the same direction.

IV. SUMMARY AND PERSPECTIVE

This work extends the reentrant phenomena to the frustrated quantum system with topological orders. We calculate the $S = 1$ antiferromagnetic Heisenberg model on a sawtooth lattice with different coupling strength parametrized by θ. The ground-state phase diagram in a magnetic field is established, where fruitful phases are revealed. By tuning the magnetic field, Haldane phase–trivial phase–partial Haldane phase transitions are observed. The partially topological-ordered phase has the coexistence of the Haldane state and topologically trivial magnetic state in the two sublattices, respectively.

In statistical physics, the reentrance is an entropic driven phenomenon, where the phase is stabilized by minimizing energy in combination with maximizing entropy [1,3–15]. The necessary condition for a reentrant phenomenon to occur is the existence of partial disordered phase with an ordered phase or a partial ordered phase [1,4]. Such a mechanism was recently extended to frustrated quantum systems at zero temperature [26], where the reentrant behavior (or the emergence of partial disorder) is a novel result of frustration and quantum fluctuations. Our work further generalizes the reentrance to topological systems, where the partially disordered phase is formed by the topological Haldane state and topologically trivial magnetic state in the two different sublattices. We expect to find more novel topological reentrant phenomena in two and higher dimensions.

Essentially, such a reentrance is to induce the topological order by adding the terms that are against the topological physics. It would be interesting to investigate the potential relations to the topological "bootstrap" that shares a same spirit, where, for instance, the $Z2$ and chiral spin liquids are induced from the free-fermion phases by adding Kondo coupling [47]. As the bond centered inversion symmetry belongs to spatial lattice symmetries, it would be also interesting to consider the partial Haldane phase as a kind of crystalline SPT [48–55].

ACKNOWLEDGMENTS

The authors acknowledge Cheng Peng, Wei Li, and Yu Chen for very useful discussions. S.-J.R. is supported by Beijing Natural Science Foundation (Grants No. 1192005 and No. Z180013) and by the Academy for Multidisciplinary Studies, Capital Normal University. S.-S.G. is supported by the National Natural Science Foundation of China (Grants No. 11834014 and No. 11874078) and the Fundamental Research Funds for the Central Universities. This work is also supported in part by the NSFC (Grant No. 11834014), the National Key R&D Program of China (Grant No. 2018FYA0305800), the Strategetic Priority Research Program of the Chinese Academy of Sciences (Grant No. XDB28000000), and Beijing Municipal Science and Technology Commission (Grant No. Z118100004218001).

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