Plateau transitions of a spin pump and bulk-edge correspondence

Yoshihito Kuno and Yasuhiro Hatsugai
Department of Physics, University of Tsukuba, Tsukuba, Ibaraki 305-8571, Japan

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Sequential plateau transitions of quantum spin chains ($S = 1, 3/2, 2$, and 3) are demonstrated by a spin pump using dimerization and a staggered magnetic field as synthetic dimensions. The bulk is characterized by the Chern number associated with the boundary twist and the pump protocol as the time. It counts the number of critical points in the loop that is specified by the Z_2 Berry phases. With an open boundary condition, the discontinuity of the spin weighted center of mass due to emergent effective edge spins also characterizes the pump as the bulk-edge correspondence. It requires extra level crossings in the pump as a superselection rule that is consistent with the valence bond solid picture.

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I. INTRODUCTION

Integer S spin systems have been extensively studied after Haldane proposed an exotic proposal for the uniform Heisenberg chains, which states the ground state is gapped if the spin is an integer [1]. Various numerical studies support this conjecture positively [2–6]. This Haldane conjecture is proved for the valence bond solid (VBS) states of the Affleck-Kennedy-Lieb-Tasaki (AKLT) model [7–9]. With open boundaries for the $S = 1$ case, there appears an extra low-energy level structure within the Haldane gap which is described by emergent effective $S = 1/2$ spins at both ends of the chain [2]. This is also consistent with the VBS picture [7–9]. The edge states were also experimentally observed [10]. According to the bulk-edge correspondence, these effective degrees of freedom are due to the nontrivial bulk [11].

This Haldane spin chain is an example of symmetry protected topological (SPT) phases [12–14]. It is robust against disorder or deformations as far as the symmetry is preserved. The SPT phase of the integer $S = 1, 2$ dimerized spin chain has been characterized by Z_2 Berry phases and is consistently understood by the VBS picture [15–19].

Recently, the topological charge pump (TCP) [20] has once again become a hot topic in the condensed matter community since recent artificial quantum systems have realized it experimentally [21–26]. The bulk-edge correspondence of the TCP has been also studied recently [27,28], although its bulk description is old. A recent field theoretical study has also discussed the generalized Berry phases related to the TCP [29]. The TCP of fermionic/bosonic systems [30–36] and the spin pump for $S = 1/2$ have been discussed [37,38], which is characterized by the Chern number [39]. Still, the nature of the spin pump for $S \geqslant 1$, especially bulk-edge correspondence, remains unclear.

In this paper, we clarify the presence of a nontrivial topological spin pump in a dimerized Heisenberg model with generic S ($S = 1, 3/2, 2$, and 3). Without using a dimensional reduction from the historical ancestor, that is, a quantum Hall system in two dimensions (2D) [24], we are proposing a nontrivial topological pump connecting two SPT phases with different edge states. We have demonstrated this spin pump by calculating the Chern number of the bulk and also discussed the low-energy spectrum of the SPT phases with small symmetry breaking parameters, that determines the behavior of the edge states during the pump. This is reflected by a series of discontinuities of the spin weighted center of mass (sCoM). Using the numerical data, we have demonstrated the bulk-edge correspondence of the generic spin chains and its relation to the VBS picture has been clarified. It suggests the inevitable existence of low-energy boundary degrees of freedom in the infinite system.

II. MODEL

In this paper, we consider a dimerized Heisenberg model with generic S [16,40], $H_{\rm DH} = \sum_{j=0}^{L-1} J_j \vec{S}_j \cdot \vec{S}_{j+1}$, $S_j^2 = S(S+1)$, where $\vec{S}_j = (S_j^x, S_j^y, S_j^z)$ and J_j is dimerized, $J_{j\in{\rm even}} = J_1$ and $J_{j\in{\rm odd}} = J_2$ [41]. The phase diagrams for $S = 1/2$ and $3/2$ [42–44] and integer cases ($S = 1$ and 2) [16,17] have been discussed before. There are sequences of gapped SPT phases denoted by SPT1, SPT2, ..., that appear by changing the ratio J_1/J_2. The schematic phase diagrams for $S = 1, 3/2$, and 2 are shown in Fig. 1. All of the SPT phases of the $H_{\rm DH}$ are protected by one of D_2, time-reversal, and bond-centered inversion symmetries [12,14,45]. The state of the SPT phases in $H_{\rm DH}$ with generic S is discussed by Z_2 Berry phases protected by the symmetry [16].

The SPT phases of the bulk are characterized by the Berry phase by a local twist [46–50], $\frac{J_2}{2}(e^{i\theta}S_0^+S_{L-1}^- + e^{-i\theta}S_0^-S_{L-1}^+)$ ($e^{i\theta} \in S^1$, $\theta \in (\pi, \pi]$). Here, we assume the sites are labeled by $i = 0, \ldots, L-1$. The Berry phase is given by $i\gamma = \int_{S^1} A_\theta(\theta)d\theta$, where $A_\theta(\theta) = \langle G(\theta)|\partial_\theta G(\theta)\rangle$ and $|G(\theta)\rangle$ is the ground state of $H_{\rm DH}(\theta)$. The SPT phases for $S = 1, 2$ are discussed and characterized by the quantized value of $\gamma = 0, \pi \in \mathbb{Z}_2$ that is consistently understood by the VBS picture

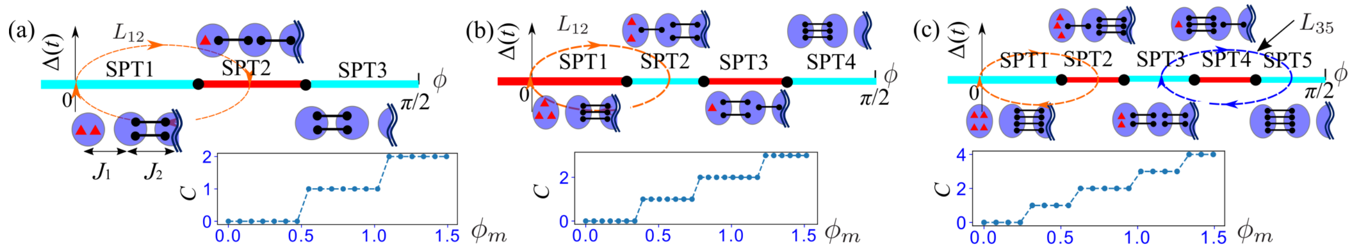

FIG. 1. (a) Schematic figures for the $S = 1$ SPT phase diagram, VBS pictures with a left open boundary, and a pump protocol in the ϕ-Δ plane. The SPT phase colored in light blue (red) has a 0 (π) Berry phase for the J_2 link. Here, $\phi = 0$ is *not* a transition point. In the VBS picture, the red triangle represents spin 1/2. The bottom panel is the plateau transition. (b) Schematic figure for the $S = 3/2$ SPT phase diagram, the VBS pictures, and a pump protocol in the ϕ-Δ plane. The bottom panel is the plateau transition. (c) Schematic figure for the $S = 2$ SPT phase diagram, and the VBS pictures. The blue loop represents the pump protocol $L_{35} = L_{15} - L_{13}$, which gives $C_{35} = C_{15} - C_{13} = 2$. The bottom panel is the plateau transition.

by assigning π for the valence bond (VB) [16,17]. Note that the gap of a finite system remains open for a system with a periodic boundary condition even near the transition points. With a twisted boundary condition, however, the gap vanishes mostly at $\theta = \pi$. It is due to the topological charge of the two bulks characterized by different Z_2 Berry phases. It suggests that extending a system by adding a $U(1) \in S^1$ twist as an associated dimension is useful for the topological transition for finite systems. This S^1 is small in the sense that the effects are infinitesimal in infinite systems [51,52]. In this sense, the transition points of the S^1-enlarged system are the same as those of the original one. Symmetry sometimes requires a gap closing for the S^1-enlarged system. The gap necessarily closes for a translationally invariant half-integer spin chain as an analog of the Lieb-Schultz-Mattis theorem for the extended system [15].

For each SPT phase in Figs. 1(a), 1(c) and 2(e), the value of γ is consistently understood by the VBS picture. Since the Berry phase has modulo 2π ambiguity, the number of bonds is specified in modulo 2. The VBS picture actually works more than that as shown later. In the topological spin pump we propose, we have observed emergent edge states predicted by the VBS picture. According to the bulk-edge correspondence, this is specified by the Chern number in the extended parameter space (see below). In the phase diagrams in Figs. 1(a), 1(c) and 1(e), all critical transition points on $\Delta = 0$ are gapless for an infinite system. Even in a finite system, the gap closes as an S^1-enlarged system.

III. TOPOLOGICAL PLATEAU TRANSITION OF A PUMP FOR A GENERIC SPIN

To characterize the ground state of $H_{\rm DH}$, let us introduce a symmetry breaking term, $H_{\rm SB} = \Delta(t)\sum_j (-1)^{j+1} S^z_j$, and consider an extended Hamiltonian $H = H_{\rm DH} + H_{\rm SB}$ where $\Delta(t)$ is a periodic dynamical parameter with a period T, which breaks *all* symmetries protecting the SPT phases. The Hamiltonian H preserves $U(1)$ symmetry of the subgroup of $SU(2)$, which implies conservation of total S^z. Here, a pump protocol is specified by a periodic modulation of the parameters. To be specific, we take $J_1(t) = \sin\phi(t), J_2(t) = \cos\phi(t)$ with $\phi(t) = \phi_m[1 - \cos(2\pi t/T)]/2$ and $\Delta(t) = \sin(2\pi t/T)$. The amplitude of the modulation ϕ_m is chosen so that the ground state of $H(t)$ at $t = 0, T/2$ (where $H_{\rm SB} = 0$) belongs to the different SPT phases as $[J_1(t), J_2(t)] = (0, 1), (\sin\phi_m, \cos\phi_m)$, $\Delta = 0$ for $t = 0$ and $T/2$, respectively. Note that the gap always remains open and the ground state is unique in the pump as for a periodic system [28].

The pump protocol is characterized by the (spin) Chern number [53] of the periodic system with a local boundary twist $e^{i\theta}$, $C = \frac{1}{2\pi i}\int_0^T dt \int_0^{2\pi} d\theta B$, where $B = \partial_\theta A_t - \partial_t A_\theta$,

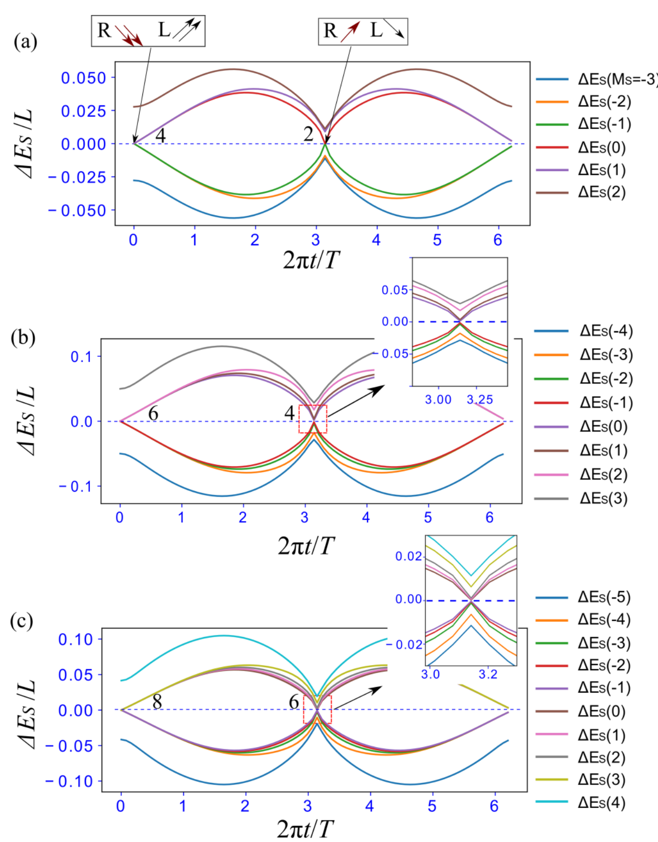

FIG. 2. (a) ΔE_S for the $S = 1$ case. We set $L = 36$. The labels "R" and "L" represent right and left edge states. The upward and downward arrows represent the direction when the edge states cross the blue dashed line. (b) ΔE_S for the $S = 3/2$ case. We set $L = 32$. (c) ΔE_S for the $S = 2$ case. We set $L = 24$. The numbers at level crossings indicate the number of the degeneracy of ΔE_S.

$A_\alpha = \langle g|\partial_\alpha g\rangle$, $\alpha = \theta, t$, where $|g\rangle$ is a gapped and unique ground state of H. The Berry phase defined at $t = 0$ and $T/2$, $|G\rangle = |g\rangle|_{\Delta=0}$, is quantized [37].

This Chern number coincides with the total pumped spin of the bulk [27,28] [see also Sec. I in the Supplemental Material (SM) [54]]. Here, let us define a Chern number, C_{1k}, for the protocol specified by the loop L_{1k} starting from the SPT1 and passing through the other kth SPT (SPTk) phases as shown in Figs. 1(a), 1(c) and 1(e). We have used the formula [55] by diagonalizing the system [56] with an even number of spins within the total $S^z \equiv \sum_{j=0}^{L-1} S_j^z = 0$ sector since the ground state is unique. The Berry phase at $t = 0$ is $2\pi S$ since the dimers are decoupled and the twist is gauged out [16]. Let us define a path $L_{kk'}$ starting from the SPTk and passing through the SPTk' and the corresponding Chern number $C_{kk'}$ [see the blue loop in Fig. 1(e) as an example]. Since the path can be deformed into the two paths L_{1k} and $L_{1k'}$ as $L_{kk'} = L_{1k'} - L_{1k}$ without a gap closing, the Chern numbers satisfy the relation $C_{kk'} = C_{k'} - C_k$.

The results of C_{1k} for the $S = 1$, $3/2$, and 2 cases are plotted in Figs. 1(b), 1(d) and 1(f) [57]. By changing the width of modulation of the dimerization ϕ_m, the Chern number changes step by step, and it is an analog of the quantum Hall plateau transitions [58–62]. The maximum Chern number for each case is $C = 2S$, that corresponds to the total number of possible dimerization transitions. The case for $S = 3$ is similar (see Sec. II in the SM [54]). The Chern number of the bulk for the pump protocol is specified by the topology of the two SPT phases where the pumps are passing through. This is clear considering a system with edges as discussed later. The gap closing points of the SPT phases on the $\Delta = 0$ line are a topological obstruction for the loop specified by the pump protocol on the ϕ-Δ plane (strictly speaking, the obstruction is for the S^1-enlarged system.) Therefore only when the loop passes through these points, is the Chern number allowed to change. The Chern number of a generic pump is given by a sum of the Chern numbers of the critical points inside the protocol loop [63]. The plateau transition of the pump in 2D is induced by the SPT transition of the 1D spin chain [64].

IV. SPIN CENTER OF MASS WITH AN OPEN BOUNDARY

Let us investigate the topological spin pump with an open boundary, especially the properties of edge states. To this end, we employ the density matrix renormalization group method in the TeNPy package [65]. We consider the sCoM [27] given by $P(t) = \sum_{j=0}^{L-1}\langle g(t)|x_j S_j^z|g(t)\rangle$, where $j_0 = (L-1)/2$, $x_j = (j - j_0)/L \in (-1/2, 1/2)$. This sCoM gives a spin current $J = \partial_t P$. Note that the sCoM is only well defined for a system with boundaries and is not well defined for a system with a periodic boundary condition. Since the pump is periodic in time, so is the sCoM, $P(t)$. It implies $0 = \int_0^T dt\, \partial_t P = \sum_i \int_{t_{i-1}}^{t_i} dt\, \partial_t P + P(t)|_{t_i-0}^{t_i+0}$, where P is piecewise continuous and has discontinuities at $t = t_i$ $(i = 1, 2, \dots)$ (periodicity in time is assumed for the summation) [27]. Then, for any path passing through SPTk and SPTk' in the parameter space, the pumped spin $Q_{kk'}^e$ in the cycle by the bulk for a system with an open boundary condition is related to the sum of the discontinuities

$$Q_{kk'}^e = \sum_i \int_{t_{i-1}}^{t_i} dt\, \partial_t P = I_{kk'}, \tag{1}$$

where $I_{kk'} \equiv -\sum_i P(t)|_{t_i-0}^{t_i+0}$.

In the spin model in this paper, each discontinuity is ± 1 which is induced by exchanging the left and right edge states [27]. It is due to the symmetry of the system. In a generic situation, single annihilation (creation) of the edge state is allowed as $P(t)|_{t_i-0}^{t_i+0} = +1/2$ at the left (right) boundary and $-1/2$ at the right (left).

We also calculate an excitation energy [38] defined by $\Delta E_S(M_S, t) = E_S(M_S + 1, t) - E_S(M_S, t)$ for each M_S sector where $E_S(M_S, t)$ is the ground state energy of H within a subspace total $S^z = M_S$. Let us discuss $\Delta E_S(M_S, t)$ at $M_S = 0, \pm 1, \dots$. We choose the same parameters as shown in the bulk calculation of Fig. 1 where the pumped spin $C_{1k} = 1$. The amplitude of the modulation ϕ_m is set to connect the SPT1 to the midpoint of the SPT2 phase ($\phi_m = \pi/4$, $3\pi/16$, and $\pi/8$ for $S = 1$, $3/2$, and 3, respectively). The results for $S = 1$, $3/2$, and 2 are shown in Figs. 2(a)–2(c). Numerically calculated excitation gaps become very small at $t = 0$ and $t = T/2$. These extremely small gaps are due to the interaction between the edge states localized near both ends of the system as emergent degrees of freedom associated with the nontrivial bulk [66]. It is an extension of the well-known effective $S = 1/2$ boundary degrees of the $S = 1$ case at $t = T/2$, that makes fourfold degeneracy in the infinite system [2]. The symmetry breaking term H_{SB} makes the degeneracy to the level crossings observed in Fig. 2. The degeneracies at $t = 0$ are trivial and are given by the addition of the bare spin S at the boundaries ($S \otimes S = 2S \oplus \cdots \oplus 0$). They are $(2S+1)^2$-fold in total and $\Delta E_S(M_S, 0) = 0$ for $4S$ different M_S sectors $M_S = -2S, \dots, 2S - 1$. Then the discontinuity at $t = 0$ is $-\sum_i P(t)|_{-0}^{+0} = 2S$.

Although the degeneracy at $t = T/2$ is nontrivial, it is consistently explained by the VBS picture [15–17]. See Figs. 1(a), 1(c) and 1(e). Based on the VBS picture, in the SPT2 phase, a single valence bond (VB) connected to the neighboring spin reduces the spin by $1/2$ at the boundary spins. It implies the effective free spins at the boundaries are $S_{\rm eff} = S - 1/2$. For the $S = 1$ case at $t = T/2$, it implies a total degeneracy of $(2S_{\rm eff} + 1)^2 = 4$ and $\Delta E_S(M_S, T/2) = 0$ for $4S_{\rm eff} = 2$ different M_S sectors. The same can be true for the SPTk phase of the spin S model where the bulk is pictorially given by the alternating $N_B^k = 2S - (k-1)$ VB on the J_2 link and $N_B^k + (k-1)$ VB on the J_1 link. The open boundary condition corresponds to cutting N_B^k VB (J_2 link), which induces effective $S_{\rm eff}^k = N_B^k/2$ spins at both ends. Then the gap closings by $\Delta E_S(M_S, T/2) = 0$ are for $4S_{\rm eff}^k = 2N_B^k = 4S - 2(k-1)$ different M_S sectors [67]. It implies that the discontinuity at $t = T/2$ is $-\sum_i P(t)|_{T/2-0}^{T/2+0} = -2S_{\rm eff}^k = -N_B^k$ (the sign is determined by the way of exchange of the left and right edge states). It contributes to the entanglement entropy by $\log(2S_{\rm eff} + 1)$ [17]. Since this effective spin is spherical due to the symmetrization according to the VBS picture.

This scenario is consistently confirmed by numerical calculations. See Figs. 2(a)–2(c). For $S = 1, 3/2$, and 2 at $t = T/2$, the degeneracies specified by ΔE_S are two-, four-, and sixfold,

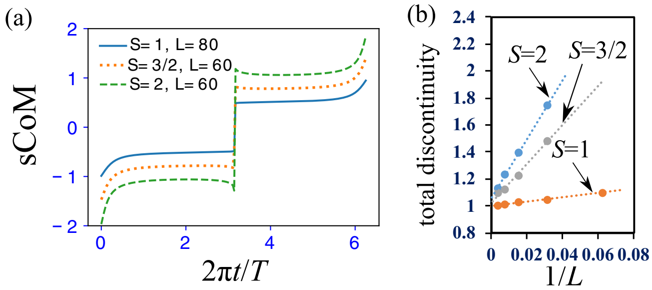

FIG. 3. (a) Behavior of the sCoM with the $S^z = 0$ sector. For the $S = 1$ case, we set $L = 80$, and for $S = 3/2$ and 2, $L = 60$. (b) System size dependence of the total discontinuity of the sCoM. It converges to an integer $I_{12} = \lim_{L\to\infty}[-\sum_i P(t)|_{t_i-\delta t}^{t_i+\delta t}]$. In the numerical calculation of the discontinuity at $t = T/2$ in the $S = 1, 3/2$, and 2 cases, we set $\delta t = 0.5 \times 10^{-2}T$, $0.5 \times 10^{-3}T$, and $0.5 \times 10^{-3}T$.

respectively. Further, for the $S = 2$ system at $t = T/2$, the level structure due to the spherical nature of the effective spin is discussed in detail (see Sec. IV in the SM [54]). Then the total discontinuity of the pump protocol starting from SPTk and passing through SPTk' is given by $I_{kk'} = N_B^k - N_B^{k'} = k' - k$. This is also consistently confirmed by numerical calculations. See Fig. 3(a), where the behaviors of sCoM of the pump for the same parameters [68] in Figs. 2(a)–2(c) are shown. For the $S = 1, 3/2$, and 2 cases, the discontinuities of $P(t = T/2)$ numerically obtained are very close to 1,2,3 ($= N_B^{k=2}$). The total discontinuity of the pump protocol starting from SPT1 ($k = 1$) and passing through SPT2 ($k' = 2$) is given by 1 ($= k' - k$). The numerical exploration to the infinite size is shown in Fig. 3(b) [69]. It implies the total discontinuity of the sCoM approaches 1 for $L \to \infty$, that is, $I_{12} = 1$.

V. BULK-EDGE CORRESPONDENCE, VBS, AND BERRY PHASES

The sCoM, $P(t)$, is a piecewise continuous function that is continuous except for several discontinuities at $t = t_i$ due to the appearance of effective boundary spins. This pumped spin by the continuous part is given by the bulk and is given by the Chern number as [27] (see also Sec. I in the SM [54]) $Q^e_{kk'} = \frac{1}{2\pi}\int_0^{2\pi} d\theta\, \bar{Q}^b_{kk'}(\theta) = C_{kk'}$, where $\bar{Q}^b_{kk'} = i\int_0^T dt\, \partial_t \bar{A}_\theta^{(t)}(\theta)$ and $\bar{A}_\theta^{(t)}$ is the Berry connection of the periodic system in the temporal gauge $\bar{A}_t^{(t)} = 0$ where the twist θ is distributed uniformly for all links. This uniform twist is transformed to the local boundary twist in the Chern number by the large gauge transformation, which makes the Chern number invariant [27,54].

Equation (1) and the representation of $Q^e_{kk'}$ imply the bulk-edge correspondence for the generic quantum spins as

$$C_{kk'} = I_{kk'} = k' - k.$$

It also imposes a constraint for the Berry phases $\gamma^k - \gamma^{k'} \equiv \pi C_{kk'}$, mod 2π. Here, we have established the bulk-edge correspondence and discussed the numerical results based on the VBS picture. Reversely, the topological stability of the Chern number implies the (fractionalized) effective $S_{\rm eff} = S/2$ free spins at both ends are topologically stable. These effective edge spins are emergent and are topologically protected by the bulk gap. This results in an inevitable level crossing of the pump with the open boundary condition as an emergent superselection rule of the infinite system.

Details of the topological pump and the bulk-edge correspondence are given in Ref. [27] and in Sec. I in the SM [54]. The large gauge transformation associated with the local $U(1)$ gauge transformation is fundamentally important.

VI. CONCLUSION

We have clarified the presence of plateau transitions and a nontrivial topological spin pump in dimerized Heisenberg models ($S = 1$, 3/2, 2, 3) with the symmetry breaking term as a synthetic dimension. The model can be feasible for a recent cold atom system [70]. The critical points between the various SPT phases are topological obstructions for the spin pump. These obstructions protect the quantization of the Chern number as the total pumped spin. Due to the bulk-edge correspondence which we have demonstrated, quantization of the Chern number implies emergent boundary degrees of freedom for the spin chains, which is consistent with the VBS picture of the dimerized Heisenberg model.

Some high-dimensional systems related to our spin pump, such as a 2D topological charge pump [72], were simulated in a recent experiment [73]. The high-dimensional extension of our spin pump is a future interesting topic. Also, an extension to the $SU(N)$ spin chains (see Refs. [50,74]) can be straightforward.

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[68] The numerical calculation of $P(t)$ is set in the $S^z = 0$ sector without the twist θ.

[69] At $t = 0$, the model is in the dimerized limit, $J_1 = 0$. Therefore, the discontinuity of the sCoM for $S = 1$, $3/2$, and 2 around

$t = 0$ with the $S^z = 0$ sector exactly becomes -2, -3, and -4, respectively.

[70] Very recently, a ladder optical lattice has realized the SPT phase [71] that can be effectively an $S = 1$ Haldane chain. The observed SPT phase is related to the one of our spin models described in this paper. It implies that our target spin Hamiltonian H and spin pump can be directly implemented and simulated by employing such a ladder optical lattice system with suitable fine tuning.

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