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Haldane topological orders in Motzkin spin chains

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Motzkin spin chains are frustration-free models whose ground state is a combination of Motzkin paths. The weight of such path contributions can be controlled by a deformation parameter t. As a function of the latter, these models, besides the formation of domain wall structures, exhibit gapped Haldane topological orders with a constant decay of string order parameters for $t < 1$. A behavior compatible with a Berezinskii-Kosterlitz-Thouless phase transition at $t = 1$ is also presented. By means of numerical calculations we show that the topological properties of the Haldane phases depend on the spin value. This allows one to classify different kinds of hidden antiferromagnetic Haldane gapped regimes associated with nontrivial features such as symmetry-protected topological order. On one hand, our results allow one to clarify the physical properties of Motzkin frustration-free chains, and on the other hand, suggest them as an interesting and paradigmatic class of local spin Hamiltonians.

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Spin chains play a crucial role in many fundamental physical phenomena such as magnetism [1], quantum phase transitions [2], topological orders [3], and quantum computation [4]. A fundamental contribution to the understanding of spin chains is provided by the seminal papers of Haldane [5], where a new topological phase, the Haldane phase (HP), uniquely detectable via a nonlocal string order parameter (SOP) [6], was discovered for spin-1 XXZ Heisenberg chains. This has driven significant efforts to look for new kinds of models whose topological order can be described in terms of a SOP [7], motivating the discovery of the celebrated Affleck-Kennedy-Lieb-Tasaki (AKLT) model [8]. Although the argument of Haldane is given for integer spin chains, only integer spin XXZ-like and AKLT-like chains have a topological HP, and it is therefore nontrivial to find and study new classes of Hamiltonians where the HP emerges. Owing to the strongest quantum "resource," namely, the entanglement, spin models also play a fundamental role in the simulation of quantum logical gates for quantum computation [4]. For this reason, finding and studying Hamiltonians with highly entangled spins is currently one of the most challenging and intriguing fields in quantum physics.

In this direction, local integer frustration-free spin Hamiltonians whose ground state can be expressed as a combination of Motzkin paths [9] have been recently introduced [10,11]. Among other interesting aspects, their importance is shown by the fact that they possess a level of entanglement entropy which strongly exceeds the one exhibited by other previously known local models. Relevantly, also for half-integer spins, a similar class of Hamiltonians, the Fredkin spin chains, exhibiting the same features [12,13], has been introduced. In addition to their entanglement properties, Motzkin chains also have very peculiar properties. Indeed, even if they are purely local models, for high spin values s (i.e., $s \geqslant 2$) they behave as *de facto* long-range Hamiltonians as they are able to violate cluster decomposition properties (CDPs) and the area law (AL) scaling of entanglement entropy [12]. Very recently, deformed versions of Motzkin [14] and of Fredkin [15] chains have been introduced, and their gaps studied [16], with the contribution of Motzkin or Fredkin paths to the ground state being weighted through the introduction of a parameter t.

Due to the aforementioned arguments it appears clear that these new models are both very interesting by themselves, and they could open the path towards fundamental applications. This motivates us to investigate a Motzkin chain for different spin values and in the presence of path deformations. Here, after an introduction of the model in terms of deformed Motzkin paths, we present density matrix renormalization group (DMRG) [17] calculations which allow one to reveal the appearance of different phases as a function of the deformation parameter t. In particular, we show that local magnetization is able to capture the $t > 1$ regime where a clear domain wall structure takes place independently by the spin value s. On one hand, once $t < 1$, the system undergoes a Berezinskii-Kosterlitz-Thouless (BKT) type phase transition [18] as signaled by an exponential opening of the gap. Moreover, our numerical calculations confirm that for this kind of deformation the entanglement entropy is bounded and size independent [14]. Crucially, we find that this gapped regime can be described solely by a nonvanishing value of SOP, thus showing the topological nature of the $t < 1$ deformed Motzkin chains. For $s = 1$ only one SOP is finite, similarly to what happens in the SU(2)-Haldane phase for XXZ or AKLT spin-1 models, thus revealing the presence of a symmetry-protected topological (SPT) order. On the other hand, for $s = 2$, different kinds of Haldane phases have been obtained [19,20]. In particular, for the spin-2 Motzkin chain, we show that two SOPs display a constant decay exhibiting a phase similar to the SO(5)-topological Haldane order occurring in the $s = 2$ AKLT model [21]. Interestingly, unlike the undeformed case $t = 1$, for $t < 1$, the CDP [22] is valid.

Model. The spin model we consider has the peculiarity of having a ground state which can be expressed in terms of Motzkin paths describing all the possible $2n$ moves that one can make go from a point of height $h = 0$ to another point of the same h without crossing the zero line

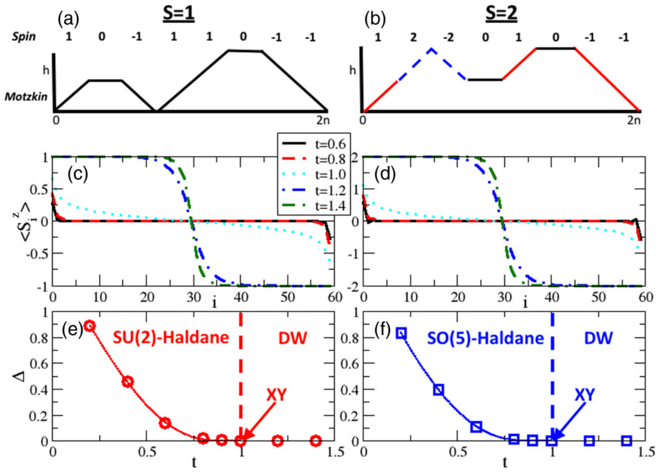

FIG. 1. Upper panels: Cartoons of a possible Motzkin path and its representation in terms of spins for the two cases: (a) uncolored $s = 1$ and (b) colored $s = 2$. Central panels: DMRG local magnetization for a system of length $2n = 60$ at different t deformation values $\langle S_i^z \rangle$ for (c) $s = 1$ and (d) $s = 2$. Lower panels: Thermodynamic limit of the gap $\Delta = E_1 - E_0$ as a function of t for (e) $s = 1$ (red circles) and (f) $s = 2$ (blue squares). The continuous lines are fitted with the form $\sim \exp(-b/\sqrt{t_c - t})$, with $t_c = 1$ and b is a fitting parameter. The thermodynamic limit is extrapolated by using chains of lengths up to $2n = 60$. All DMRG simulations are performed by keeping at most 1024 DMRG states and five finite size sweeps with an error energy $<10^{-9}$ (10^{-7}) for $s = 1$ $(s = 2)$.

[10,11]. As shown in Figs. 1(a) and 1(b), spins can be seen as moves by imposing that up/zero/down spin corresponds to increasing/conserving/decreasing the height of the path. Of course, for spin $s = 1$ only uncolored steps (uncolored Motzkin chain) are allowed, while larger values of s can be achieved when colored steps are possible (colored Motzkin chain). The Hamiltonian reads

$$H = \sum_{j=1}^{2n-1} \Pi_{j,j+1}(s,t) + \Pi_\partial(s) + \sum_{j=1}^{2n-1} \Pi_{j,j+1}^{\text{cross}}(s), \qquad (1)$$

where $\Pi_{j,j+1}(s,t) = \sum_{k=1}^{s} (|\phi(t)^k\rangle\langle\phi(t)^k|_{j,j+1} + |\psi(t)^k\rangle\langle\psi(t)^k|_{j,j+1}| + |\Theta(t)^k\rangle\langle\Theta(t)^k|_{j,j+1})$ is the bulk term, and $\Pi_\partial(s) = \sum_{k=1}^{s} |-k\rangle\langle -k|_1 + |k\rangle\langle k|_{2n}$ is the boundary term which makes it more favorable for the first spin to point upward, $|k\rangle$, and the last downward, $|-k\rangle$. The latter term in Eq. (1), $\Pi_{j,j+1}^{\text{cross}}(s) = \sum_{k\neq k'} = |k,-k'\rangle\langle k,-k'|$, present only for $s > 1$, ensures the color matching of up and down spins with the same h. The parameter t appearing in $\Pi_{j,j+1}(s,t)$ describes path deformations and $|\phi(t)^k\rangle = (1+t^2)^{-1/2}(|k,0\rangle - t|0,k\rangle)$, $|\psi(t)^k\rangle = (1+t^2)^{-1/2}(|0,-k\rangle - t|-k,0\rangle)$, and $|\Theta(t)^k\rangle = (1+t^2)^{-1/2}(|k,-k\rangle - t|0,0\rangle)$. The deformation induced by $t \neq 1$ keeps the model frustration free [14], and, while for $t = 1$ we recover the undeformed model [10–12], for $t > 1$ $(t < 1)$ the paths having larger (smaller) h are favored in the ground state. Notice that, for $t = 1$, one can have analytical expressions for the magnetization and the z-z correlation functions, which were tested against DMRG results in Ref. [12]. However, for $t \neq 1$, the corresponding results are not available and therefore we will rely on DMRG results to have a physical description of the properties of the model.

$t \geqslant 1$ regime. This latter point explains the $t > 1$ behavior of the local magnetization $\langle S_j^z \rangle$ observed in Figs. 1(c) and 1(d) for $s = 1$ and $s = 2$, respectively. Indeed, since $t > 1$ makes higher paths more probable, in terms of spins this corresponds to a domain wall (DW) structure where the up and down spins are separated in two different regions of equal length n [23] and the zero spins are basically absent. Relevantly, as shown in Figs. 1(e) and 1(f), this latter regime is gapless $(\Delta = 0)$, meaning that the difference between the ground state E_0 and the first excited state E_1 energy goes to zero in the thermodynamic limit (TDL). The aforementioned features allow one to find the analogy between Eq. (1) and the XXZ chains for both spin 1 and 2 [24] for strong negative z anisotropies. Further similarities can be also noticed for the $t = 1$ case where a gapless regime is associated with a power-law decay of the correlation function $\langle S_i^+ S_j^- \rangle$ and, as exactly shown in Ref. [12], an exponential decay of $\langle S_i^z S_j^z \rangle - \langle S_i^z \rangle\langle S_j^z \rangle$ [25], thus resembling the XY phase of XXZ models, but with the key feature that both AL decay and CDP are violated for $s = 2$.

$t < 1$ regime. On one hand, as already mentioned, a $t < 1$ deformation minimizes the height of the possible paths. This is clearly visible in the $\langle S_j^z \rangle$ behavior shown in Figs. 1(c) and 1(d) where an almost totally flat local magnetization with $h = 0$ is observed. Crucially, $\langle S_j^z \rangle$ shows also antiparallel peaks at the edges of the chain, thus supporting the possible presence of edge states. This effect, as explained before, is produced by the $\Pi_\partial(s)$ term in Eq. (1), which also plays the role of breaking the ground-state degeneracy. The almost flat magnetization can also explain the fact that the entanglement entropy, $S(A) = -\mathrm{Tr}\, \rho_A \log_2 \rho_A$ of a subsystem A, is bounded and does not depend on either the chain or on the partition length [14], meaning that the AL scaling is fulfilled. Indeed, as it is possible to see in Fig. 2(a), we find that $S(A)$ is constant at fixed t for any $2n$ while it grows almost linearly with the deformation strength. The latter is easily explained by the fact that, for $t < 1$, the strength of t actually affects mainly the first and the last move with flat $\langle S_j^z \rangle = 0$ in the bulk. Consequently, a larger (smaller) t will produce a higher (lower) value of $|\langle S_i^z \rangle|$ in the first and last site, as shown in Fig. 1, thus generating more (less) entropy, which is, however, size independent (see the inset in the top panel of Fig. 2) because of the flatness of the paths that mainly contribute to the ground state. Notice that, as shown in Fig. 2(a), this behavior holds for any s value considered. A less trivial aspect, conjectured in Ref. [14], emerges by looking at Figs. 1(e) and 1(f), namely, $t < 1$ deformations support the presence of a finite gap in the TDL. As is visible in the same figures, for both $s = 1$ and $s = 2$, the gap opens compatibly with an exponential decay $\Delta \sim \exp(-b/\sqrt{t_c - t})$, where $t_c = 1$ and b is a fitting parameter, thus signaling a BKT-like phase transition. In integer spin chains, the gapped regime can be usually associated with either an antiferromagnetic (AF) order described by the two-point correlation functions

$$C(|i-j|) = \langle S_i^z S_j^z \rangle - \langle S_i^z \rangle\langle S_j^z \rangle, \qquad (2)$$

or with Haldane orders described by a SOP,

$$O^{k,\bar{k}}(|i-j|) = \langle L_i^{k,\bar{k}} e^{\imath\pi \sum_{i\leqslant \ell < j} L_\ell^{k,\bar{k}}} L_j^{k,\bar{k}} \rangle, \qquad (3)$$

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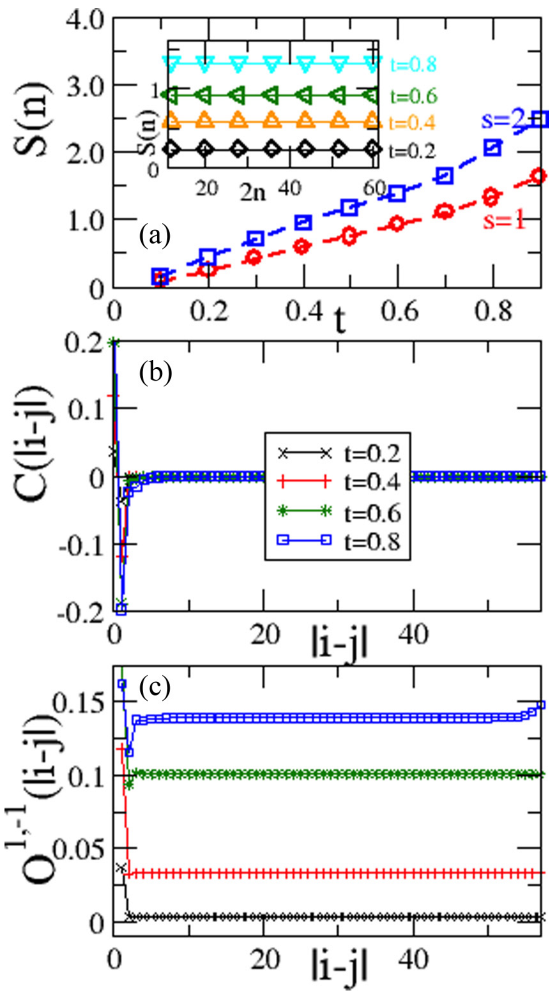

FIG. 2. (a) Entanglement entropy $S(A)$ for a subsystem having length n with $1 \leqslant i \leqslant n$ for $s = 1$ (red symbols) and $s = 2$ (blue symbols). The inset shows the constant behavior of $S(A)$ as a function of size $2n$. (b) $C(|i-j|)$ for different $t < 1$ values. (c) $O^{1,-1}(|i-j|)$ for different $t < 1$ values. The correlations in (b) and (c) are evaluated in a system of size $2n = 60$ with i pinned in the first chain site. We checked that different i values do not alter the physical behavior of the correlations.

where $L^{k,\bar{k}} = |k\rangle\langle k| - |-k\rangle\langle -k|$. Notice that, for $s = 1$, $k(\bar{k})$ can be solely equal to $1(-1)$, thus $L_i^{1,-1} = S_i^z$, while for $s = 2$, $k(\bar{k})$ can take the values $1(-1)$ and $2(-2)$ and $S_i^z = 2\,L_i^{2,-2} + L_i^{1,-1}$. The important information encoded in such nonlocal order parameters is that, once it is finite, Eq. (3) describes a topological phase, usually called HP, with a hidden antiferromagnetism (HAF). The HAF order is given by the fact that it cannot be described by the usual two-point correlation functions Eq. (2) thus describing a phase where spins up and down are rigorously alternated and separated by a random number of zero spins. Of course, while for $s = 1$ the HP can be given only by alternating $+1$ and -1 spins thus signaled by a finite $O^{1,-1}(|i-j|)$, for $s = 2$, the hidden order can be signaled, as it will be clear in the following, by two or even solely one finite $O^{k,\bar{k}}(|i-j|)$.

$s = 1$ case. Here, we start our analysis of the $s = 1$ case by evaluating both $O^{1,-1}(|i-j|)$ and $C(|i-j|)$ for different $t < 1$ values. Figure 2 clearly shows that while $C(|i-j|)$ rapidly decays to zero, the SOP remains constant as a function of distance, thus signaling the presence of a HP. This aspect, in analogy with XXZ chains, supports our prediction regarding the BKT nature of the phase transition. We also checked that the SOPs along transverse directions decay. Furthermore, as visible in Fig. 2(c), $O^{1,-1}(|i-j|)$ saturates to a constant value which becomes bigger the larger is t. At first glance this aspect could seems counterintuitive since one expects that the larger the gap, the stronger is the SOP. Nevertheless, an easy interpretation of the $O^{1,-1}(|i-j|)$ behavior as a function of t comes from the geometrical meaning of the deformations. Indeed, as explained before, a small t favors paths with low h. Intuitively, one can argue that the path with smaller h is the one where the first and last moves correspond to respectively the rising and the lowering steps with a series of flat moves in the middle. This means that the number of $+1$, -1 spins producing the HAF order is minimized by reducing t, thus producing a lower saturation value of the SOP. Nevertheless, we checked that even very small deformations support the presence of a constant $O^{1,-1}(|i-j|)$, suddenly disappearing $[O^{1,-1}(|i-j|) = 0]$ for $t = 1$, thus allowing one to unambiguously conclude that the uncolored $t < 1$ Motzkin chain has a topological order with HAF. This phase is usually called the SU(2)-Haldane phase and it has been observed in both spin-1 XXZ [6,26] chains and in the AKLT model [27]. We will keep this nomenclature even if for our model only the operator $\sum_i S_i^z = \sum_i L_i^{1,-1}$ commutes with the Hamiltonian. This is similar to what happens in the spin-1 XXZ model when a single ion anisotropy term is included, breaking the SU(2) invariance but preserving the HP. For certain systems such as the spin-1 XXZ model, the topological order is also captured by an even degeneracy of the entanglement spectrum (ES) [28]. On the other hand, in different models, such as, for instance, the AKLT [29] or exotic bosonic Hamiltonians [30], the ES does not present an even degeneracy, but the topological order is assured by the presence of edge modes and finite SOPs. We checked that this happens also in our case where the ES of $t < 1$ deformed Motzkin chains does not display any degeneracy. Nevertheless, the edge modes, visible in Figs. 1(c) and 1(d), and the finite SOP in Fig. 2 assure the topological order [31]. The latter has a further fundamental property due to fact that it appears for an odd value s of the spin. Indeed, once a HP takes place for odd spins s, SPT order [7] is generated. This is given by the fact that the edge modes fractionalize in two half-integer spins which cannot be removed unless they are in the presence of a phase transition or an explicit symmetry breaking. This consideration allows one to conclude that the $s = 1$ version of Eq. (1) with $t < 1$ deformations supports the presence of SPT topological order with bounded and size-independent entanglement thus strongly characterizing the Motzkin chains.

$s = 2$ case. As shown in Refs. [11,12], the $s > 1$ undeformed $t = 1$ chains have many more intriguing properties with respect to the lower spin case. These are induced by the presence of colors which increase the symmetry of the system. As for the $s = 1$, $s = 2$ XXZ Heisenberg and AKLT models can support the presence of gapped phases for positive z anisotropies. The gap can again be associated with the AF order detected by $C(|i-j|)$ or to different kinds of HP (see, for instance, Refs. [19,32] and references therein). In particular,

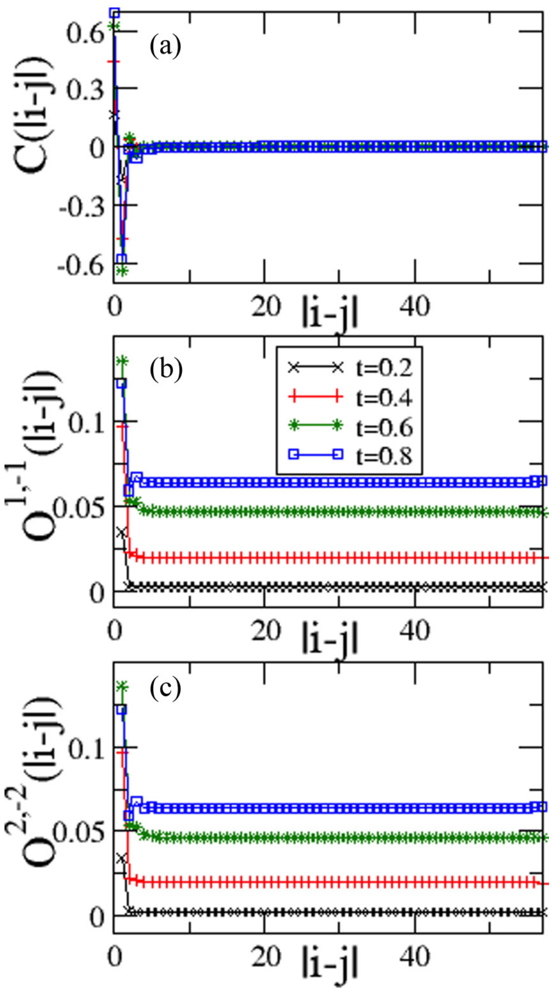

FIG. 3. (a) $C(|i-j|)$ for different $t<1$ values. (b) $O^{1,-1}(|i-j|)$ for different $t<1$ values. (c) $O^{2,-2}(|i-j|)$ for different $t<1$ values. All the correlations are evaluated in a system of size $2n=60$ with i pinned in the first chain site. We checked that using different values of i does not alter the physical behavior of the correlations.

in such systems, SPT topological order is signaled by finite values of both $O^{1,-1}(|i-j|)$ and $O^{2,-2}(|i-j|)$. Moreover, as conjectured in Ref. [33] and shown in Refs. [32,34], single ion anisotropy terms can support the formation of a SPT SU(2)-Haldane order even for $s=2$. Our calculations in Fig. 1(f) show that again the colored Motzkin chain is gapped for $t<1$ and the gap is associated with HAF since $C(|i-j|)$ has a clear exponential decay rapidly saturating to zero, as shown in Fig. 3(a). On the other hand, both $O^{1,-1}(|i-j|)$ and $O^{2,-2}(|i-j|)$ have a constant and basically equal behavior, thus clarifying that the $s=2$ Motzkin chains with $t<1$ deformations support the presence of an SO(5)-HP. It is worth stressing that SO(5) is not the symmetry of our model, rather $U(1)\times U(1)\times\mathbb{Z}_2$, since only $\sum_i L_i^{2,-2}$ and $\sum_i L_i^{1,-1}$ commute with the Hamiltonian, as in the $s=2$ AKLT model when the term $\sum_i (S_i^z)^2$ is switched on. Also, in that case, the SO(5)-Haldane phase survives once the symmetry is lowered from SO(5) to $U(1)\times U(1)$ [35]. In our case the symmetry is supplemented by the invariance under interchanging the two colors ($\mathbb{Z}_2$). This is the reason why $O^{1,-1}(|i-j|)$ and $O^{2,-2}(|i-j|)$ are the same, as shown in Fig. 3. Moreover, it is important to notice that, in analogy with the $s=1$ case, the SOPs become stronger with increasing t. Figure 3(b) also shows more information encoded in the $C(|i-j|)$ behavior. Indeed, contrary to the $t=1$ regime [12], its exponential decay is associated with a zero edge-to-edge value, thus holding the CDP. The opening of a gap in a colored Motzkin chain therefore restores the pure locality of the model in Eq. (1), in agreement with the general findings for gapped local Hamiltonians [36].

Conclusions and perspectives. In conclusion, our results demonstrate the existence of topological Haldane orders in a different class of spin Hamiltonians. Furthermore, we have shown the behavior of Motzkin chains as a function of the deformation strength t. While the undeformed $t=1$ case has XY-like features, for $t>1$, the system presents a gapless domain wall structure. On the other hand, at $t=1$, we presented evidence of a BKT-like phase transition, characterized by an exponential opening of the gap, occurring for any $t<1$ values. The gapped regime is associated with SPT-hidden Haldane antiferromagnetic orders signaled by finite values of string nonlocal order parameters. The two possible Haldane orders have the peculiarity of having an entanglement entropy independent of both block and chain size. Moreover, our results suggest that it would be very interesting to have a physical implementation of the Motzkin spin chains. In this respect, cold atomic systems, which have been already proposed to simulate several kinds of spin Hamiltonians with topological orders [37], could provide a possible physical platform to implement Motzkin chains. Their experimental realization could be relevant for technological achievements since, on one hand, symmetry-protected topological orders have been proposed as ideal candidates towards the realization quantum devices such as quantum repeaters [38] and substrates for measurement-based quantum computation [39], while, on the other hand, Motzkin paths may have applications in the field of polymer absorption [40]. Finally, we underscore that, in future works, it would be very interesting to study the gapped regimes in the fermionic version of the $s=3/2$ Fredkin model where exotic Haldane regimes can take place [41].

Note added. Recently, we became aware of work where a Motzkin spin chain is considered by introducing a field theory approach to study certain observables and entanglement measures [42]. We think that addressing the properties discussed in the present Rapid Communication by such an approach would be very interesting, in particular, the discussion on the BKT nature of the transition at $t=1$.

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