A parent Hubbard model for spin-1 Haldane chains

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The Haldane phase for antiferromagnetic spin-1 chains is a celebrated topological state of matter, featuring gapped excitations and fractional spin-1/2 edge states. Here we provide numerical evidence that this phase can be realized with a Hubbard model at half-filling, where each \( s = 1 \) spin is stored in a four-site fermionic structure. We find that the noninteracting limit of our proposed parent model describes a one-dimensional topological insulator, adiabatically connected to the Haldane phase. Our work suggests a route to build spin-1 networks using Hubbard model quantum simulators.

The emergence of physical properties that are absent in the building blocks of interacting quantum systems is a central theme of condensed matter physics. Fractionalization, a phenomenon whereby the collective excitations of a system have quantum numbers that cannot be obtained from its elementary constituents, provides a powerful evidence of the 	extit{more is different} paradigm \cite{1}.

One of the simplest models that features fractionalization is the Heisenberg Hamiltonian for spin-1 chains with nearest-neighbor antiferromagnetic (AF) interactions \( S_i \cdot S_{i+1} \) (where \( S_i \) denotes the vector of spin-1 operators at site \( i \)). In contrast to the spin-1/2 counterparts, Haldane predicted \cite{2,3} that one-dimensional (1D) spin-1 Heisenberg antiferromagnets with 	extit{periodic boundary conditions} should have a gapped excitation spectrum, along with a singlet ground state for which the spin-spin correlation function decays exponentially.

The seminal work of Haldane was later backed up by the analytical valence bond solid solution of the Affleck–Kennedy–Lieb–Tasaki (AKLT) model \cite{4}, where Haldane’s conjecture was rigorously verified for the 1D AF spin-1 Haldane Hamiltonian with additional nearest-neighbor biquadratic terms \( \beta S_i \cdot S_{i+1}^2 \), taking \( \beta = 1/3 \). Remarkably, the AKLT solution for 	extit{open boundary conditions} revealed a fourfold degenerate ground state due to the emergence of two fractional spin-1/2 degrees of freedom at the chain edges.

Further numerical work \cite{5,6} established that the generalization of the AKLT Hamiltonian for arbitrary \( \beta \), hereafter referred to as the bilinear-biquadratic (BLBQ) model, features both the gapped excitations and the fractional spin-1/2 edge states, with a fourfold degeneracy in the thermodynamic limit, in a range of \( \beta \) that includes \( 0 \leq \beta \leq 1/3 \). We refer to this as the Haldane phase.

The connection between the nature of the boundary conditions and the ground state degeneracy is a hallmark of topological order. In the case of spin-1 Haldane chains, it has been shown that a hidden form of topological AF order, akin to that of the fractional quantum Hall effect \cite{7} and intimately related to a symmetry breaking \cite{8}, can be detected through nonlocal string order parameters \cite{9,10}. It is now understood that the Haldane phase is a symmetry-protected topological phase \cite{11,12}.

In this manuscript, we present a 	extit{parent} Hubbard model that captures the Haldane physics of spin-1 BLBQ chains. We consider a Hubbard Hamiltonian at half-filling, defined in a 1D lattice with four sites per unit cell, and show, by numerical means, that its low-energy properties are well described by a BLBQ model in the Haldane phase, thereby connecting two celebrated milestones \cite{13,14} of the last half-century. Furthermore, we find that our proposed parent Hamiltonian interpolates between a spin-1 Haldane chain for \( U > 0 \) (where \( U \) denotes the on-site Hubbard repulsion) and a 1D topological insulator in the noninteracting limit \( U = 0 \).

Early work showed that the Haldane phase can be obtained in spin-1/2 Heisenberg alternating chains \cite{15} and ladders \cite{17,18} with all couplings of the AF type. Given that, in the limit of large \( U \), the Hubbard model at half-filling is known to map into a spin-1/2 AF Heisenberg Hamiltonian \cite{19}, this opens a way to realize the Haldane physics with Fermi-Hubbard systems \cite{20}. It must also be noted that, by turning off the interactions of a variety of fermionic models in the Haldane phase, both trivial \cite{21,22} and topological \cite{23,24} 1D band insulators have been adiabatically retrieved. In contrast to the aforementioned literature, here we put forward a Hubbard Hamiltonian that exhibits fractional spin-1/2 edge states supported in four-site fermionic structures that are robust \( s = 1 \) spins, effectively generated for any \( U > 0 \) without the need of additional terms.

The first key step of our strategy to realize the Haldane physics with a Hubbard model is to generate a robust \( s = 1 \) spin. Inspired by previous work \cite{25,26}, we propose the 	extit{four-site cluster}—a fermionic structure with trigonal planar geometry in which the three outer sites
are linked to the central one via an intrachain hopping \( t > 0 \) (Fig. 1b). The four-site cluster is bipartite and has a sublattice imbalance of \( |N_A - N_B| = 2 \) (where \( N_{A/B} \) denotes the number of sites of the \( A/B \) sublattice) which implies, by virtue of Lieb’s theorem [27], that the corresponding Hubbard model at half-filling must yield a ground state with total spin \( S = 1 \). Moreover, exact diagonalization of the model yields a splitting \( \Delta \) between the \( S = 1 \) ground state and the first excited state, as a function of \( U \), obtained with the Hubbard model for the four-site cluster at half-filling.

The next step toward the realization of the Haldane phase is to create a 1D lattice of antiferromagnetically coupled \( s = 1 \) four-site clusters. We first consider the case of \( N = 2 \) chains (where \( N \) denotes either the number of four-site clusters or the number of \( s = 1 \) spins), which we refer to as *dimers*. To achieve an effective AF coupling in the four-site dimer, we introduce an intercluster hopping \( t' > 0 \) between the closest sites of each of the two four-site clusters (Fig. 2a). We find that, for small enough \( t' \)—which preserves the picture of robust spin-1 building blocks (see the Supplemental Material for technical details on how the upper bounds of \( t' \) are set)—, the four-site Hubbard dimer at half-filling yields a low-energy spectrum that can be matched, spin degeneracies included, to that of the BLBQ model with an effective energy spectrum that can be matched, spin degeneracies.

are expected to be smaller than \( \Delta \), as previously anticipated. This ascertains that the four-site clusters, albeit coupling antiferromagnetically, have a large effective superexchange scaling [19].

To provide further evidence that our proposed 1D four-site Hubbard lattice at half-filling captures the Haldane physics of spin-1 BLBQ chains, we now extend the comparison between both models for chains with \( N > 2 \) (Fig. 3), keeping the same \( J \) and \( \beta \) as obtained for the dimer. We use the QUSpin package [28] to perform exact diagonalization on spin-1 BLBQ chains up to \( N = 19 \) (the limit within our computational resources), and the iTensor library [30] for density matrix renormalization group [31, 32] calculations on \( N \geq 20 \) spin-1 BLBQ chains and \( N \geq 3 \) four-site Hubbard lattices.

Figure 3 shows the five lowest energy levels obtained with both Hubbard and BLBQ models for \( N = 10 \) chains, using different sets of model parameters. An overall agreement is apparent, with differences verified to be smaller than \( J/10 \) for all the energy levels. We also observe that, whereas the pattern of spin degenera-

**FIG. 1**: Four-site cluster as a robust spin-1 building block. (a) Representation of a four-site cluster as an \( s = 1 \) spin. Colors of small circles denote the two sublattices. (b) Energy splitting between the \( S = 1 \) ground state and the first excited state, as a function of \( U \), obtained with the Hubbard model for the four-site cluster at half-filling.

**FIG. 2**: Effective spin picture of two coupled four-site clusters. (a) Depiction of a four-site dimer as an AF spin-1 dimer with bilinear \((J)\) and biquadratic \((\beta J)\) exchange couplings. (b, c) BLBQ model parameters \( J \) (b) and \( \beta \) (c), as a function of the Hubbard model parameters, obtained by matching the energy levels of the spin-1 BLBQ dimer to the low-energy spectrum of the four-site Hubbard dimer at half-filling.
cies is the same no matter the model parameters taken, the agreement between the energies is worse when $\beta$ is larger. This suggests that higher-order corrections, such as bicubic exchange couplings, should be included if a better quantitative description is sought.

Now that the low-energy spectra of both Hubbard and BLBQ models was shown to hold a good agreement, we move on to the comparison of other wave function properties. For that matter, we define the correlator

$$g_{\mathcal{O},\mathcal{U}}(d) = \left\langle \mathcal{O}_p \left( \prod_{q=p+1}^{p+d-1} \mathcal{U}_q \right) \mathcal{O}_{p+d} \right\rangle,$$

where $\mathcal{O}_p$ and $\mathcal{U}_p$ are arbitrary local operators that act on site $p$, assumed to be sufficiently away from the edges, so that $g_{\mathcal{O},\mathcal{U}}(d)$ is independent of $p$. Notably, the spin-string correlator $|g_{S^z, R^z}(d)|$, where $R^z_p = \exp(i\pi S^z_p)$, is known to be an order parameter that, when evaluated for a state in the fourfold ground state manifold of spin-1 Haldane chains, converges to a finite value $37$ ($|g_{S^z, R^z}(\infty)| \simeq 0.37$ in the case of the Heisenberg model $6$). On the other hand, the pure-string correlator $|g_{s, R^z}(d)|$ has been established as an order parameter that, for the same state, exhibits the opposite behavior, vanishing in the $d \gg 1$ limit $10$. For comparison purposes, given that each four-site cluster is mapped into an $s = 1$ spin, in the case of the Hubbard model we take the local spin operators as the sum of fermionic spin operators over the corresponding four-site clusters, i.e.,

$$\hat{S}_i = \frac{1}{2} \sum_{j \in \text{cluster}_i} \left( \hat{c}_{j,\uparrow}^{\dagger} \hat{c}_{j,\downarrow}^{\dagger} + \hat{c}_{j,\downarrow} \hat{c}_{j,\uparrow} \right) \cdot \boldsymbol{\tau} \cdot \left( \hat{c}_{j,\uparrow}^{\dagger} \hat{c}_{j,\downarrow} \right),$$

where $\boldsymbol{\tau}$ is the vector of Pauli matrices and $c_{j,\sigma}^{\dagger}$ ($\hat{c}_{j,\sigma}$) is the creation (annihilation) operator for an electron in site $j$ with spin $\sigma = \uparrow, \downarrow$.

In Fig. 3a-g, we present expectation values and correlators computed for the lowest energy state with $|S, S_z\rangle = |1, +1\rangle$ of $N = 50$ four-site Hubbard and spin-1 BLBQ chains, using the same model parameters as in (c).
both models capture the Haldane physics, as the string order parameters \( \langle g_{z,R}(d) \rangle \) and \( \langle g_{1,R}(d) \rangle \) are shown to follow the characteristic behaviors [9,10]. Notably, both models yield a striking agreement in all these calculations, thus supporting our claim of its equivalence.

For completeness, we have verified that the Hubbard-BLBQ mapping holds not only for \( U = t \) (Fig. 3), but for all \( U > 0 \). In the Supplemental Material, we show calculations for \( U = 0.1t \), relevant to connect with the noninteracting limit, and for \( U = 10t \), in which case the Hubbard model effectively maps into a spin-1/2 Heisenberg Hamiltonian [19]. It must be noted that the magnitude of \( U \) determines the spin-1 robustness of the four-site clusters (quantified by \( \Delta \)), with the main consequence being that a maximal \( \Delta \) allows for a maximal \( J \), a scenario that occurs for \( U \approx 3t \) (Fig. 1b) [53]. Besides that, in the Supplemental Material we also show that the C\(_3\) symmetry of the four-site clusters is not a necessary requirement for the Hubbard-BLBQ mapping to hold.

We now consider the \( U = 0 \) limit of the four-site 1D lattice. As in the interacting case, we take \( t' \ll t \). Figure 1a shows the energy bands of the four-site 1D crystal \( (N \to \infty) \), which feature a gap at half-filling. We find that the low-energy bands possess a Zak phase of \( \pi \) [54], known to be a topological marker for 1D insulators with inversion symmetry [33]. Expectedly [34], we also find that chains with finite length host two in-gap states localized at the edges (Fig. 1b,c). Interestingly, these states have rigorously zero-energy regardless of \( N \) (Fig. 1b) [54] and are strictly localized at two edge sites (Fig. 1c), in contrast, for instance, to the topological edge states of the Su-Schrieffer-Heeger model [35]. We associate the zero-energy states obtained with our model to a symmetry that consists in interchanging the two dangling sites of each edge [39].

Finally, we conjecture a topological equivalence between the \( U = 0 \) limit of the four-site 1D lattice at half-filling, shown to describe a topological insulator, and the \( U > 0 \) regime, that realizes the Haldane symmetry-protected topological phase, according to our computations. Our conjecture is based on two points. First, in both cases the ground state is unique for periodic boundary conditions and degenerate for open-ended chains. Second, Hubbard interactions are not expected to close the \( U = 0 \) gap and therefore it is possible to adiabatically deform the \( U = 0 \) limit into the \( U > 0 \) regime.

In conclusion, we have shown that a Hubbard Hamiltonian at half-filling, defined in a 1D lattice that hosts effective \( s = 1 \) spins at each of its four-site unit cells, realizes the Haldane phase. The proposed strategy opens a way to engineer spin-1 Haldane chains, as well as other layouts, through a variety of physical systems that are being explored for quantum simulation of the Hubbard model, such as cold atoms [37,38], quantum dots [39,40], dopant arrays [41], hydrogenated graphene bilayers [42] and spin-1/2 networks [43,44]. Our findings pave the way to new experiments, going beyond early seminal works [45,47], as well as the recent observations on triangulene spin chains [29]. Additional interest comes from the fact that both the AKLT ground state and its spin-3/2 counterpart on a honeycomb lattice are resources for measurement-based quantum computing [48,49].

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\[ J \approx A - B \sum_{i=0}^{n-1} \left( \frac{t}{U} \right)^{n-i} \delta_{i,k} \]