

Instability of the Haldane phase: Roles of charge fluctuations and Hund's coupling

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 (Received 8 July 2025; revised 17 September 2025; accepted 19 September 2025; published 1 October 2025)

We systematically investigate the stability of the symmetry-protected topological (SPT) Haldane phase in spin- $\frac{1}{2}$ Heisenberg and half-filled Hubbard ladders coupled by ferromagnetic Hund's interactions. Using the density-matrix renormalization group method, we analyze key signatures of the Haldane phase: long-range string order, finite spin gap, and characteristic entanglement spectrum degeneracies. In spin-only Heisenberg ladders, we find immediate onset and continuous strengthening of the Haldane phase with increasing Hund's coupling. In contrast, the inclusion of charge fluctuations in Hubbard ladders leads to a nontrivial stability regime, revealing a robust yet bounded region where SPT order persists despite significant charge fluctuations. We identify distinct boundaries separating a trivial insulating phase from the Haldane SPT phase, governed by both Coulomb repulsion and Hund's coupling. Our results highlight the subtle interplay of spin and charge degrees of freedom in correlated itinerant systems and establish essential criteria for observing Haldane physics experimentally in fermionic ladder materials.

DOI: [10.1103/8h2q-4wnt](https://doi.org/10.1103/8h2q-4wnt)

Introduction. Understanding the robustness of topological phases in the presence of competing interactions and additional degrees of freedom remains a central challenge in condensed matter physics. Symmetry-protected topological (SPT) phases, exemplified by the Haldane phase [1,2] in spin-1 chains, exhibit hallmark features including a finite spin gap [3,4], nonlocal string order [5–7], and fractionalized edge states [8,9] protected by discrete symmetries [10–13]. While these properties have been thoroughly established for idealized spin-only models, their stability in realistic materials featuring significant charge fluctuations and orbital degrees of freedom remains poorly understood and is a highly nontrivial issue [14].

Initially, experimental realization of the Haldane phase occurred predominantly in transition-metal oxides [15–19]. More recently, synthetic quantum systems such as metal-organic frameworks [20], organic molecular chains [21], and ultracold atomic ladders [22] have demonstrated essential characteristics of the Haldane phase, thereby prompting critical new questions regarding its robustness under reduced electron correlations and enhanced charge fluctuations. Resolving the stability and topological integrity of the Haldane phase in these realistic contexts is thus pivotal both for fundamental insights into quantum magnetism and for guiding the development of novel topological quantum materials.

Recent theoretical investigations have focused intensively on the robustness of SPT phases in specialized fermionic ladder systems, especially regarding the Haldane phase [23–26]. These studies underscore the crucial roles played by orbital degeneracy, charge dynamics, and symmetry protection. Nevertheless, a comprehensive, quantitative understanding of how charge fluctuations, governed specifically by Coulomb repulsion and Hund's coupling, affect the stability or potential breakdown of the Haldane phase is still lacking.

In this Letter, we systematically investigate the stability of the SPT Haldane phase by performing density-matrix renormalization group (DMRG) [27] calculations on two complementary ladder models: a Heisenberg ladder to clarify the role of Hund's coupling and a Hubbard ladder to elucidate the effects of charge fluctuations as well as Hund's coupling. We accurately determine the phase boundaries separating the SPT Haldane phase from a trivial Mott/Hund insulating phase, explicitly demonstrating the breakdown of the Haldane phase under sufficiently strong charge fluctuations. Clarifying these conditions is crucial not only for a deeper understanding of correlated topological phases but also as foundational groundwork for exploring unconventional superconductivity and spin-singlet pairing in doped Haldane systems [28–33].

Model definitions and effective mapping. We consider two models of coupled one-dimensional (1D) chains with interchain ferromagnetic (FM) Hund's coupling: a spin- $\frac{1}{2}$ Heisenberg ladder and a half-filled Hubbard ladder. The Heisenberg ladder serves as a spin-only reference system, while the latter incorporates charge degrees of freedom and their fluctuations.

The Heisenberg ladder is described by

$$H_{\text{Heis}} = J \sum_{\gamma=1,2} \sum_i \mathbf{S}_{\gamma,i} \cdot \mathbf{S}_{\gamma,i+1} - J_H \sum_i \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i}, \quad (1)$$

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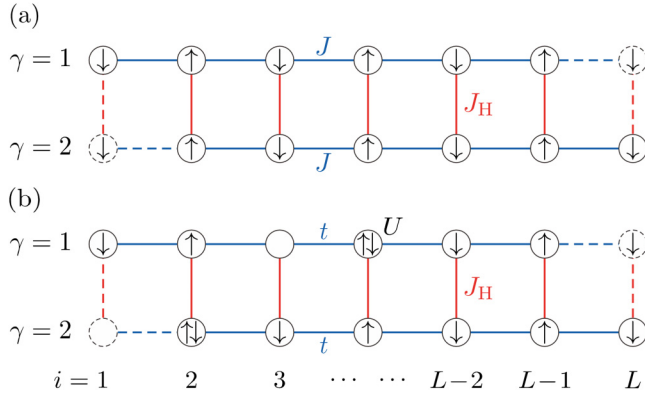


FIG. 1. Lattice structures of (a) the two-leg Heisenberg ladder and (b) the two-leg Hubbard ladder, with FM Hund's coupling J_H connecting the chains. Indices γ and i label the leg and site positions, respectively. Removing the dashed bonds corresponds to replacing the edge spins with spin- $\frac{1}{2}$ degrees of freedom in the effective spin-1 Heisenberg chain representation.

where $\mathbf{S}_{\gamma,i}$ denotes a spin- $\frac{1}{2}$ operator on leg γ and site i , $J > 0$ is the antiferromagnetic (AFM) intrachain coupling, and $J_H > 0$ is the FM Hund's coupling along the rungs. The corresponding Hubbard ladder is given by

$$H_{\text{Hub}} = -t \sum_{\gamma=1,2} \sum_{i,\sigma} (c_{\gamma,i,\sigma}^\dagger c_{\gamma,i+1,\sigma} + \text{H.c.}) + U \sum_{\gamma,i} n_{\gamma,i,\uparrow} n_{\gamma,i,\downarrow} - J_H \sum_i \mathbf{S}_{1,i} \cdot \mathbf{S}_{2,i}, \quad (2)$$

where $c_{\gamma,i,\sigma}^\dagger$ ($c_{\gamma,i,\sigma}$) creates (annihilates) a fermion with spin σ on leg γ and site i , t is the intrachain hopping amplitude, and U is the on-site Coulomb repulsion. Schematic illustrations of the ladder geometry are shown in Fig. 1.

In the Heisenberg ladder (1), the FM Hund's coupling favors the formation of rung triplets. The low-energy Hilbert space is then approximately restricted to the spin-triplet subspace on each rung [34]: $|1\rangle_i = |\uparrow\rangle_{1,i} |\uparrow\rangle_{2,i}$, $|0\rangle_i = (|\uparrow\rangle_{1,i} |\downarrow\rangle_{2,i} + |\downarrow\rangle_{1,i} |\uparrow\rangle_{2,i})/\sqrt{2}$, and $|-1\rangle_i = |\downarrow\rangle_{1,i} |\downarrow\rangle_{2,i}$. Projecting onto this subspace yields an effective spin-1 Heisenberg chain:

$$H_{\text{eff}} = \frac{J}{2} \sum_i \tilde{\mathbf{S}}_i \cdot \tilde{\mathbf{S}}_{i+1} - \frac{J_H}{4} L, \quad (3)$$

where $\tilde{\mathbf{S}}_i = \mathbf{S}_{1,i} + \mathbf{S}_{2,i}$ is a spin-1 operator on rung i and L is the number of rungs. This emergent spin-1 mechanism differs from materials with intrinsic local spin-1 ions (e.g., Ni^{2+}), yet at low energies the two are adiabatically connected and realize the same Haldane SPT phase, as elaborated in the Supplemental Material [35].

A similar mapping is expected for the Hubbard ladder at large U/t and/or J_H/t . In this regime, charge fluctuations are suppressed: the on-site repulsion U penalizes double occupancy, while FM Hund's coupling J_H favors rung spin-triplet formation, stabilizing effective spin-1 moments. Although the precise coupling range for the validity of this spin-only mapping is not known, complete suppression of charge fluctuations is not necessary; dominance of rung triplet states

suffices. This provides a controlled platform to explore how residual charge fluctuations impact SPT order.

Numerical methods and observables. We perform extensive DMRG simulations on open ladders with up to $L \times 2 = 241 \times 2$ sites, keeping up to $\chi = 10\,000$ density-matrix eigenstates. To characterize the Haldane phase, we calculate four key observables: the string correlation function, spin gap, entanglement spectrum (ES), and spin-spin correlation functions. Numerical values are extrapolated carefully to $\chi \rightarrow \infty$ where necessary.

The string correlation function is defined as

$$\mathcal{O}_{\text{str}}(i, j) = \left\langle \tilde{\mathbf{S}}_i^z \exp \left(i\pi \sum_{k=i+1}^{j-1} \tilde{\mathbf{S}}_k^z \right) \tilde{\mathbf{S}}_j^z \right\rangle, \quad (4)$$

whose asymptotic value $|\mathcal{O}_{\text{str}}(-\infty, \infty)|$ serves as the string order parameter. In practice, when the order is robust, $|\mathcal{O}_{\text{str}}(i, j)|$ rapidly reaches a flat plateau as $|i - j|$ increases on large open ladders; in this case we read off the plateau value from a fixed, sufficiently long ladder and take it as the order parameter. When the plateau is not unambiguous (e.g., near phase boundaries), we determine the order parameter by finite-size scaling of a central estimator evaluated on $L \times 2$ ladders (see the Supplemental Material for details [35]). For the spin-1 Heisenberg chain, this parameter takes the value $|\mathcal{O}_{\text{str}}^{S=1}(-\infty, \infty)| \approx 0.3743$ [4,36].

The spin gap is obtained from the singlet-triplet excitation energies, defined as $\Delta_s = \lim_{L \rightarrow \infty} [E_0(L, 1) - E_0(L, 0)]$, where $E_0(L, S^z)$ is the ground-state energy of a ladder with L rungs and total spin S^z along the z axis. To eliminate zero-energy excitations associated with spin- $\frac{1}{2}$ edge states, we remove one spin- $\frac{1}{2}$ site from each ladder edge, leaving effective spin- $\frac{1}{2}$ degrees of freedom on the outermost rungs (see Fig. 1). The spin gap for the spin-1 Heisenberg chain [Eq. (3)] is well established as $\Delta_s^{S=1}/J = 0.205\,239\,62$ [4,37,38].

Additionally, we examine the ES [39], obtained from the Schmidt decomposition of the ground state upon bipartitioning: $|\Psi\rangle = \sum_\alpha \lambda_\alpha |\phi_\alpha^L\rangle \otimes |\phi_\alpha^R\rangle$. The eigenvalues λ_α^2 of the reduced density matrix $\rho_L = \text{Tr}_R |\Psi\rangle\langle\Psi|$ define the ES. In the Haldane phase, the ES displays characteristic evenfold degeneracies, directly indicating fractionalized spin- $\frac{1}{2}$ edge states and confirming SPT order.

Haldane phase in the Heisenberg ladder. We first investigate how the Heisenberg ladder converges to the effective spin-1 Heisenberg chain [Eq. (3)] as J_H/J increases. Figure 2(a) shows the string correlation function $|\mathcal{O}_{\text{str}}(i, j)|$ versus distance $|i - j|$ for several values of J_H/J , computed on a 193×2 ladder. For all J_H/J values considered, the correlation function clearly saturates at large distances, confirming robust long-range string order.

In Fig. 2(b), we plot the extracted string order parameter as a function of J_H/J . As J_H/J grows, the string order parameter continuously approaches the known spin-1 Heisenberg chain value, demonstrating that the ladder progressively realizes the effective spin-1 limit. As shown in the inset, the string order parameter follows the scaling form $|\mathcal{O}_{\text{str}}(i, j)| \propto \sqrt{J_H/J}$ in the small- J_H/J regime, indicating the immediate onset of the Haldane phase for any finite $J_H > 0$. Consistent with this, the

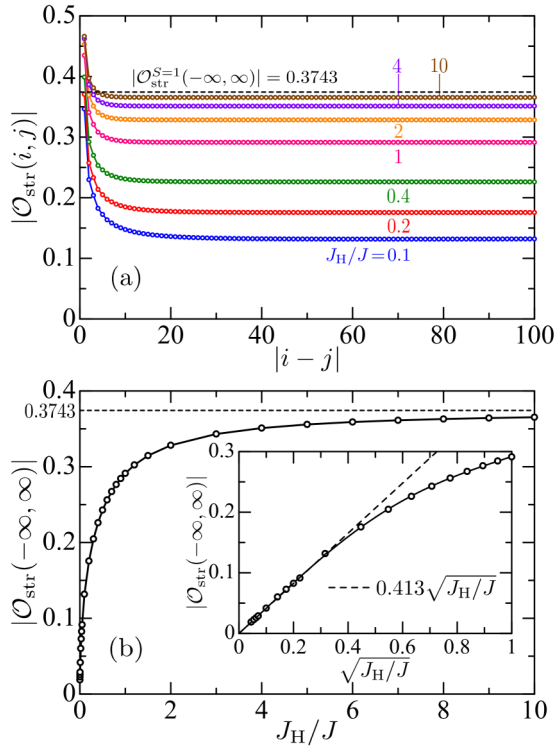


FIG. 2. String order in the Heisenberg ladder. (a) String correlation function $\mathcal{O}_{\text{str}}(|i - j|)$ plotted as a function of distance $|i - j|$ for several values of J_H/J . The dotted line indicates the string order parameter of the $S = 1$ Heisenberg chain. (b) String order parameter $|\mathcal{O}_{\text{str}}(-\infty, \infty)|$ as a function of J_H/J . Inset: $|\mathcal{O}_{\text{str}}(-\infty, \infty)|$ plotted against $\sqrt{J_H/J}$ in the small J_H/J regime; the dashed line shows a fit near $J_H/J = 0$.

spin gap opens simultaneously with the emergence of string order, as discussed in detail below.

Charge fluctuations in the Hubbard ladder. We now turn to the Hubbard ladder [Eq. (2)], which differs from the Heisenberg ladder by allowing double occupancy of lattice sites, thereby introducing charge fluctuations. To quantify these fluctuations, we examine the local charge variance, defined as $\delta n^2 = \langle n_{\gamma,i}^2 \rangle - \langle n_{\gamma,i} \rangle^2$. At half filling, this quantity directly relates to double occupancy: $\delta n^2 = 2\langle n_{\gamma,i,\uparrow} n_{\gamma,i,\downarrow} \rangle$.

Figure 3 shows δn^2 as a function of t/U and t/J_H . Increasing U naturally reduces double occupancy, suppressing δn^2 and pushing the system toward the spin-only limit. Increasing J_H similarly suppresses charge fluctuations, but through a distinct mechanism: FM Hund's coupling energetically favors rung spin-triplet formation, thereby stabilizing well-defined spin- $\frac{1}{2}$ states and disfavoring doublon-holon pairs. Consequently, δn^2 decreases systematically. Thus Coulomb repulsion U and Hund's coupling J_H cooperatively reduce charge fluctuations, stabilizing an effective low-energy spin description.

Topological order in the Hubbard ladder. We now investigate how charge fluctuations influence topological order in the Hubbard ladder by examining the string correlation function $\mathcal{O}_{\text{str}}(i, j)$. Figure 4(a) presents $|\mathcal{O}_{\text{str}}(i, j)|$ as a function of distance $|i - j|$ for several values of J_H/t at fixed $U/t = 4$, while Fig. 4(b) shows similar results for various U/t at fixed

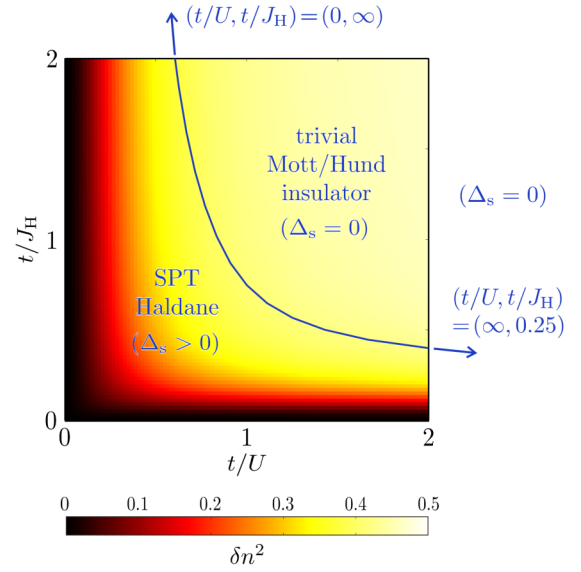


FIG. 3. Charge fluctuations in the Hubbard ladder. Local charge variance δn^2 plotted as a function of t/U and t/J_H . The solid line indicates the phase boundary separating the trivial Mott/Hund insulating phase from the topological Haldane phase.

$J_H/t = 4$, computed on a 97×2 ladder. In both cases, the string correlation saturates at finite values at large distances, confirming robust long-range order. With increasing U/t or J_H/t , charge fluctuations are progressively suppressed, driving the system closer to the effective spin-1 regime. Correspondingly, the saturated value, i.e., the string order parameter, approaches the spin-1 Heisenberg chain value. Thus the Hubbard ladder can realize a stable Haldane phase despite moderate charge fluctuations.

However, when both U/t and J_H/t are small and charge fluctuations dominate, the string correlations vanish at large distances, signaling the absence of long-range string order. Figure 4(c) shows a log-log plot of $|\mathcal{O}_{\text{str}}(i, j)|$ versus distance for equal interaction strengths $U/t = J_H/t$. At weak coupling ($U/t = J_H/t = 1$), a power-law decay is observed, indicating no long-range order. At stronger coupling ($U/t = J_H/t = 2$), however, finite long-range string order emerges, signaling a topological phase transition between these two interaction strengths. Notably, near the critical point, the string order parameter grows nearly linearly, unlike the square-root behavior observed in the Heisenberg ladder, before gradually approaching the spin-1 Heisenberg chain value at stronger interactions.

Long-range string order appears even at $U/t = 0$, driven solely by Hund's coupling. Figure 4(d) shows log-log plots of the string correlation for various J_H/t values at zero on-site repulsion. A clear transition from power-law decay ($J_H/t = 3$) to finite long-range order ($J_H/t \geq 6$) is observed, reflecting strong suppression of charge fluctuations (double occupancy) by Hund's coupling alone. This insulating phase stabilized purely by Hund's coupling can thus be viewed as a novel ‘‘Hund insulator.’’ The string order parameter, shown in Fig. 4(f), grows around $J_H/t \approx 4.0$, approaching the spin-1 Heisenberg value at large J_H/t , again following an approximately linear onset.

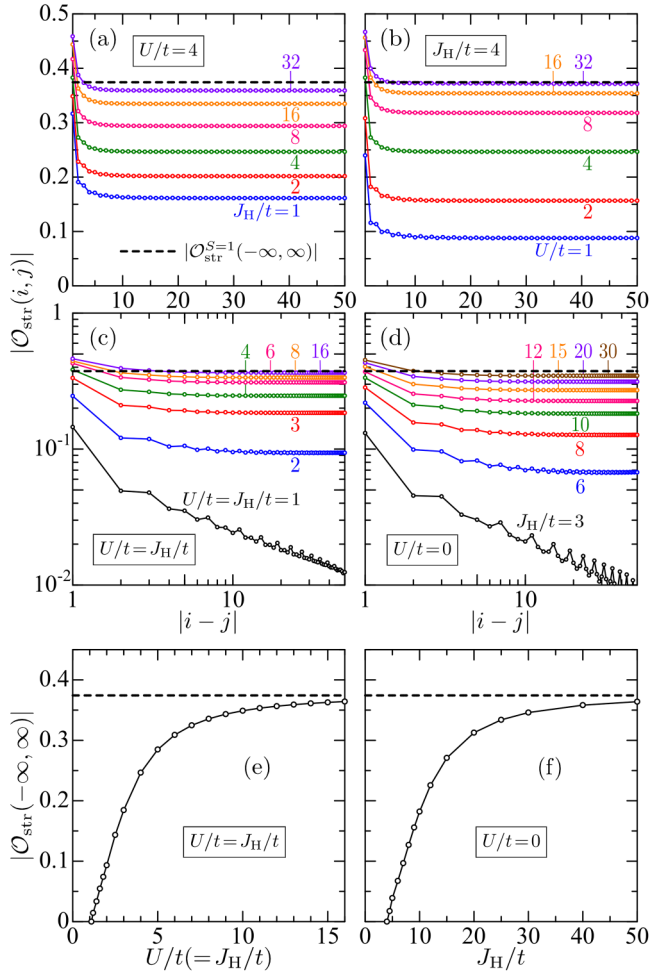


FIG. 4. Topological string order in the Hubbard ladder. String correlation function $O_{\text{str}}(i, j)$ versus $|i - j|$ for (a) various J_H/t at fixed $U/t = 4$ and (b) various U/t at fixed $J_H/t = 4$. Log-log plots of $O_{\text{str}}(i, j)$ versus $|i - j|$ for (c) various interaction strengths with $U/t = J_H/t$ and (d) various J_H/t at fixed $U/t = 0$. String order parameter as a function of (e) $U/t = J_H/t$ and (f) J_H/t at fixed $U/t = 0$. Dotted lines mark the spin-1 Heisenberg chain value.

The resulting phase diagram, summarized in Fig. 3, reveals a clear boundary between the trivial Mott/Hund insulating phase and the SPT Haldane phase, identified explicitly by the string order parameter. Notably, the Haldane phase remains stable under substantial charge fluctuations, persisting up to a local charge variance of approximately $\delta n^2 = 2\langle n_{\gamma, i, \uparrow} n_{\gamma, i, \downarrow} \rangle \lesssim 0.4$. Furthermore, the phase boundary approaches $J_H = 0$ in the $U = \infty$ limit, indicating a smooth crossover from the Hubbard to the Heisenberg ladder in the strongly correlated regime. Although our model setup is different, the qualitative agreement with the topological transition line reported in Ref. [26] supports the broader conclusion that the Haldane phase is generally stable against moderate charge fluctuations.

Spin gap and edge states. A finite spin gap is a defining feature of the Haldane phase. To confirm its presence, we compute the spin gap Δ_s , first considering the Heisenberg ladder. Figure 5(a) shows the spin gap Δ_s/J versus J_H/J . Consistent with the immediate onset of string order, a spin gap

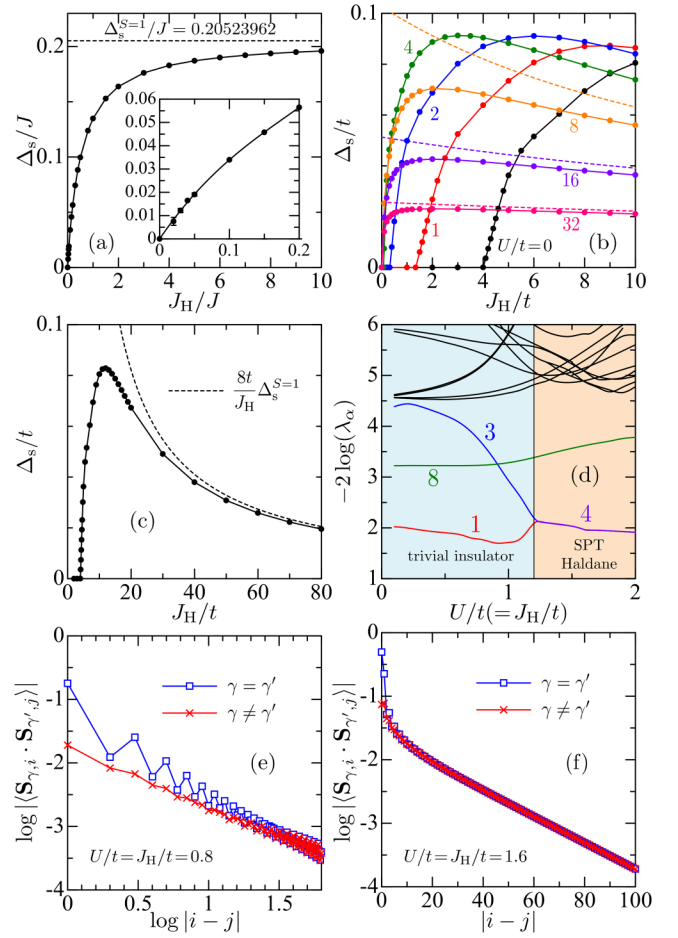


FIG. 5. (a) Spin gap Δ_s/J for the Heisenberg ladder as a function of J_H/J . The dashed line marks the spin gap of the spin-1 Heisenberg chain [Eq. (3)]. Inset: enlarged view of the small- J_H/J region. (b) Δ_s/t for the Hubbard ladder as a function of J_H/t for several values of U/t . (c) Δ_s/t as a function of J_H/t at $U = 0$. Dashed lines in (b) and (c) indicate strong-coupling estimates. (d) Entanglement spectrum across the topological transition at $U/t = J_H/t \approx 1.2$. Numbers beside the lines denote entanglement level degeneracies. (e), (f) Spin-spin correlation function $\langle S_{\gamma, i} \cdot S_{\gamma', j} \rangle$ as a function of distance r , shown on (e) log-log and (f) semilog scales for $U/t = J_H/t = 0.8$ and 1.6 , respectively.

emerges immediately upon introducing finite J_H , confirming that the Haldane phase appears throughout the entire $J_H > 0$ regime. At small J_H/J , the gap grows approximately linearly, contrasting the singular, square-root onset of the string order. In the large- J_H/J limit, the gap approaches the known spin-1 Heisenberg chain value $\Delta_s^{S=1}/J = 0.20523962$.

The relationship between spin gap and string order in the Hubbard ladder is more subtle. Figure 5(b) plots Δ_s/t as a function of J_H/t for various U/t . A finite spin gap exists broadly, disappearing only at small U/t and J_H/t . A strong-coupling analysis yields an effective exchange $J_{\text{eff}} = 4t^2/(U + J_H/2)$, predicting the asymptotic behavior $\Delta_s/t = \{4t/(U + J_H/2)\} \Delta_s^{S=1}$. Also, a finite gap persists even at $U/t = 0$ for $J_H/t \gtrsim 4$, reflecting an effective repulsion generated purely by strong Hund's coupling [Fig. 5(c)]. Here, the gap asymptotically follows $\Delta_s/t = (8t/J_H) \Delta_s^{S=1}$. Details of

the strong-coupling analysis are given in the Supplemental Material [35].

Overlaying the finite spin-gap region onto Fig. 3, we find a perfect match with the finite string-order region. This nontrivial correspondence strongly supports the identification of this regime as a genuine Haldane phase. We also find that slightly away from half filling both the nonlocal string order and the spin gap remain finite in the infinitesimal doping limit (see the Supplemental Material [35]).

To further confirm the topological character, we analyze the ES. Figure 5(d) shows the ES across the topological transition at $U/t = J_H/t \approx 1.2$. The lowest entanglement level is nondegenerate in the trivial insulating phase, becoming fourfold degenerate immediately upon entering the Haldane phase, consistent with the expected SPT order.

Finally, we examine real-space spin correlations to further distinguish the gapped Haldane phase from gapless trivial states. Figures 5(e) and 5(f) present intra- and interleg spin correlations $\langle \mathbf{S}_{\gamma,i} \cdot \mathbf{S}_{\gamma',j} \rangle$ as functions of distance $|i - j|$. In the Haldane phase ($U/t = J_H/t = 1.6$), the correlations decay exponentially as $\langle \mathbf{S}_{\gamma,i} \cdot \mathbf{S}_{\gamma',j} \rangle \sim \exp(-|i - j|/\xi)$ ($\xi > 0$), whereas, in the gapless regime ($U/t = J_H/t = 0.8$), correlations show power-law decay, signaling criticality. Notably, within the Haldane phase, intra- and interleg correlations rapidly coincide, validating the emergence of effective spin-1 degrees of freedom and reinforcing the

interpretation of the ladder as an effective spin-1 chain at low energies.

Summary. We have investigated the stability of the Haldane phase in Heisenberg and Hubbard ladders with interchain Hund's coupling. While the Heisenberg ladder realizes a spin-1 Haldane phase for any finite $J_H > 0$, the inclusion of charge fluctuations in the Hubbard ladder leads to qualitatively distinct behavior. Using DMRG simulations, we demonstrated that the Haldane phase—characterized by long-range string order, a finite spin gap, and degeneracies in the ES—persists over a broad parameter range in the Hubbard ladder, but ultimately breaks down when both U and J_H are small.

These results establish that the Haldane phase remains robust against moderate charge fluctuations, but is destabilized when electronic itinerancy becomes too strong. Our findings highlight the subtle interplay between spin and charge degrees of freedom in realizing SPT phases and delineate the conditions under which topological order can persist in correlated itinerant systems.

Acknowledgments. We thank U. Nitzsche for technical assistance. This project is funded by the German Research Foundation (DFG) via Project A05 of the Collaborative Research Center SFB 1143 (Project-id No. 247310070). Part of the DMRG calculations in this work were performed using the ITensor Software Library [40].

Data availability. The data that support the findings of this Letter are openly available [41].

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