## Hubbard model for spin-1 Haldane chains

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The Haldane phase [1] for antiferromagnetic spin-1 chains is a celebrated topological state of matter, featuring gapped excitations and fractional spin-1/2 edge states. Here [2], 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 (Fig. 1). We find that the noninteracting limit of our proposed model describes a one-dimensional (1D) topological insulator, and we conjecture it to be adiabatically connected to the Haldane phase. Our work opens a way to engineer spin-1 Haldane chains, as well as other spin networks, through a variety of physical systems that are being explored for quantum simulation of the Hubbard model [3,4]. We also show that our proposed Hubbard model accurately describes the observation of fractionalization in nanographene triangulene chains [5].

## References

- [1] F. D. M. Haldane, Phys. Rev. Lett., 50 (1983) 1153.
- [2] G. Catarina, J. Fernández-Rossier, Phys. Rev. B, 105 (2022) L081116.
- [3] T. Hensgens, T. Fujita, L. Janssen, X. Li, C. J. Van Diepen, C. Reichl, W. Wegscheider, S. Das Sarma, L. M. K. Vandersypen, Nature, 548 (2017) 70.
- [4] A. Mazurenko, C. S. Chiu, G. Ji, M. F. Parsons, M. Kanász-Nagy, R. Schmidt, F. Grusdt, E. Demler, D. Greif, M. Greiner, Nature, 545 (2017) 462.
- [5] S. Mishra, **G. Catarina**, F. Wu, R. Ortiz, D. Jacob, K. Eimre, J. Ma, C. A. Pignedoli, X. Feng, P. Ruffieux, <u>J. Fernández-Rossier</u>, R. Fasel, Nature, 598 (2021) 287.



**Figure 1:** (a) Sketch of the general mapping between a 1D Hubbard lattice, with hoppings *t* and *t'*, and an antiferromagnetic spin-1 chain, with bilinear (*J*) and biquadratic ( $\beta J$ ) exchange couplings (BLBQ model), where *N* four-site fermionic structures are mapped into *N s*=1 spins. (b) Comparison between the lowest-energy levels of *N*=10 four-site Hubbard and spin-1 BLBQ chains, with the corresponding total spin *S* indicated. Hubbard model results were obtained at half filling, for a Hubbard repulsion *U*=*t*, with *t'*=0.06*t*. BLBQ model parameters *J*=2.51×10<sup>-3</sup>*t* and  $\beta$ =1.91×10<sup>-2</sup> were fixed by matching the low-energy spectra of *N*=2 chains. (c) Average magnetization and (d) string order parameters, obtained for the lowest-energy state with |*S*,*S*<sub>2</sub>>=|1,+1> of *N*=50 four-site Hubbard and spin-1 BLBQ chains, using the same model parameters as in (b). The agreement between both models is apparent. The observation of spin-1/2 edge fractionalization (c), vanishing pure-string (d, inset) and nonvanishing spin-string (d) correlators are indicative of the spin-1 Haldane phase.

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