Investigation of the chiral antiferromagnetic Heisenberg model using PEPS

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A simple spin-1/2 frustrated antiferromagnetic Heisenberg model (AFHM) on the square lattice – including chiral plaquette cyclic terms – was argued [Anne E.B. Nielsen, Germán Sierra and J. Ignacio Cirac, Nature Communications 4, 2864 (2013)] to host a bosonic Kalmeyer-Laughlin (KL) fractional quantum Hall ground state [V. Kalmeyer and R. B. Laughlin, Phys. Rev. Lett. 59, 2095 (1987)]. Here, we construct generic families of chiral projected entangled pair states (chiral PEPS) with low bond dimension ($D = 3, 4, 5$) which, upon optimization, provide better variational energies than the KL ansatz. The optimal $D = 3$ PEPS exhibits chiral edge modes described by the Wess-Zumino-Witten $SU(2)_1$ model, as expected for the KL spin liquid. However, we find evidence that, in contrast to the KL state, the PEPS spin liquids have power-law dimer-dimer correlations and exhibit a gossamer long-range tail in the spin-spin correlations. We conjecture that these features are genuine to local chiral AFHM on bipartite lattices.

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Introduction. Topological order (TO) has been rationalized in the last few decades [1, 2] as a new type of order in two dimensions (2D), beyond the well-known Ginzburg-Landau paradigm. Importantly, it is at the heart of the rapidly expanding field of quantum computing [3]. The fractional quantum Hall (FQH) state of the 2D electron gas [4] is the first topological ordered state discovered. The simple Laughlin wave function provides a beautiful qualitative understanding of the physics of the Abelian FQH state at filling fraction $\nu = 1/m$ as an incompressible fluid [5], while more involved wave functions can also describe non-Abelian FQH states [6-8]. It revealed the emergence of fractional excitations, the anyons, a key feature of TO [1]. Anyons carry fractional charge [5] as well as Abelian [9] or non-Abelian statistics [6, 10]. An important feature of FQH states is the existence of a bulk gap and chiral modes providing unidirectional transport on the edge [11, 12]. More precisely, their edge physics can be described by chiral $SU(2)_k$ Wess-Zumino-Witten (WZW) Conformal Field Theory (CFT) [13]. Recently, a matrix product state (MPS) representation of the FQH states [14, 15] enabled to probe their physical properties with unprecedented numerical accuracy.

In a pioneering work [16], Kalmeyer and Laughlin (KL) have extended the notion of FQH state to the lattice. When localized on the lattice, the bosonic $\nu = 1/2$ Laughlin state gives rise to a spin-1/2 chiral spin liquid (CSL) [17], closely related to the resonating valence bond (RVB) state of high-Tc superconductivity [18]. Recently, fractional Chern insulators [19-21] have set up a new route to realize FQH physics on the lattice.

Whether simple local lattice Hamiltonians can host chiral spin liquid ground states [17] is one of the key issues that determine whether or not such topological phases could be realized experimentally. The original innovative proposal by KL that the GS of the frustrated triangular spin-1/2 antiferromagnetic Heisenberg model (AFHM) is a CSL turned out not to be correct, the GS of this model being magnetically ordered. However, Bauer et al. [23] showed recently that, on the kagome lattice (2D lattice of corner-sharing triangles), the GS of the Hamiltonian $H = \sum_{\Delta(ijk)} S_i \cdot (S_j \times S_k)$, sum of the chiral spin interaction over all triangles $\Delta(ijk)$, has the universal properties of the $\nu = 1/2$ Laughlin state. This CSL was shown to be exceptionally robust under the addition of an extra nearest-neighbor Heisenberg-like interaction (defining a generic “chiral AFHM”), even of large magnitude.

Another alternative approach has been pursued, trying to construct “parent Hamiltonians” for the Abelian [24, 25] and non-Abelian [26, 27] CSL. Using a re-writing...
TABLE I. Numbers of independent $SU(2)$-symmetric tensors for the four different virtual spaces we consider, $D \leq 5$. The third (fourth) column gives the number of $A_1$ ($A_2$) tensors and the last column the total number of tensors in the $A$ ansatz. Note that all four types of ansätze exhibit a gauge-$Z_2$ symmetry associated to the conserved parity of the number of spin-$\frac{1}{2}$ on the $z = 4$ bonds.

| $V$   | $D$  | $A_1^{(A_1)}$ | $A_2^{(A_2)}$ | Total # |
|-------|------|---------------|---------------|---------|
| $\frac{1}{2} \oplus 0$ | 3    | 2             | 1             | 3       |
| $0 \oplus 0 \oplus 0$ | 4    | 8             | 4             | 12      |
| $\frac{1}{2} \oplus 0$ | 5    | 10            | 8             | 18      |
| $\frac{1}{2} \oplus 0 \oplus 0 \oplus 5$ | 21   | 12            | 33           |         |

of the wave function as a correlator of a $1 + 1$ chiral CFT [28, 29], the simplest spin-$\frac{1}{2}$ parent Hamiltonian on the square lattice obtained by Nielsen et al. [22] consists of interactions between all pairs and triples of spins in the system. Since long-range interactions might be hard to achieve experimentally in e.g. cold atom systems [30], the authors argue that a similar (Abelian) CSL phase is also hosted in a simplified local Hamiltonian where all the long-range parts of the interaction have been set to zero [22]. We shall adopt here their local chiral AFHM which, introducing a slightly different parametrization, reads:

$$H = J_1 \sum_{i,j} \mathbf{S}_i \cdot \mathbf{S}_j + J_2 \sum_{k,l} \mathbf{S}_k \cdot \mathbf{S}_l + \lambda_c \sum_{ijkl} i(P_{ijkl} - P_{ijkl}^{-1}),$$

(1)

where the first (second) sum is taken over nearest-neighbor (next-nearest-neighbor) bonds and the last sum over all plaquettes of the square lattice. $P_{ijkl}$ makes a cyclic permutation of the four spins of each plaquette in e.g. the clockwise direction. $H$ breaks time reversal symmetry but preserves the global spin $SU(2)$ symmetry. It is the analog for the square lattice of the sal symmetry but preserves the global spin in e.g. the clockwise direction.

Our strategy to explore the physics of the above model is to use the tensor network framework [31–35]. One of the motivation is to test whether some fundamental obstruction is at play that prevents to describe a gapped CSL phase with 2D tensor networks [36]. Previous attempts using projected entangled pair states (PEPS) led to the discovery of critical CSL exhibiting chiral edge modes [37–39]. PEPS are ansätze that approximate GS wave functions in terms of a unique site tensor $A_{\alpha \beta \gamma \delta}$, where the greek indices label the states of the $D$-dimensional virtual spaces $V$ attached to each site in the $z = 4$ directions of the lattice, and $s = \pm \frac{1}{2}$ is the $S_z$ component of the physical spin. The site tensors are then entangled together (i.e. contracted w.r.t. their virtual indices) to form a 2D tensor network. A priori, all the $2^D$ coefficients of the site tensor can serve as parameters to optimize the variational GS energy. However, the CSL bears a number of symmetry properties that greatly constrains the PEPS ansatz. Recently, a classification of fully $SU(2)$-symmetric (singlet) PEPS was proposed [40] in terms of the irreducible representations (IRREP) of the lattice point group ($C_{4v}$ in the case of the 2D square lattice). Since the CSL should be invariant under the combination of a reflection $R$ w.r.t. to any crystalline direction $(x, y, x \pm y)$ and time reversal symmetry (i.e. complex conjugation), the simplest adequate PEPS site tensors have the form $A = A^{(A_1)}_R + iA^{(A_2)}_R$, where the two real tensors $A^{(A_1)}_R$ and $A^{(A_2)}_R$ transform according to the $A_1$ (symmetric w.r.t. $R$) and $A_2$ (antisymmetric w.r.t. $R$) IRREP [38, 39]. These tensors have been tabulated in Ref. 40 for $D \leq 6$, and their numbers for all virtual spaces $V$ considered in this work are listed in Table I. Following a previous study of the non-chiral frus-

![Fig. 2.](image-url) [Color online] Scaling of the iPEPS variational energies (per site) vs $D^2/\chi$ for the two local chiral Hamiltonians studied here; (a) $J_1 - \lambda_c$ model; (b) $J_1 - J_2 - \lambda_c$ model. The filled (open) symbols correspond to fully optimized (fixed) tensors as explained in the text. A comparison with the exact energy (per site) of a $5 \times 6$ torus [22] is shown. In (b) the variational energy of the Kalmeyer-Laughlin (KL) spin liquid obtained by Monte Carlo [22] is also shown.
trated AFHM [41], we consider a general superposition of all tensors of each class, the weights in the sum being considered as variational parameters. As in the non-chiral case, the energy or observables can be computed directly in the thermodynamic limit using infinite-PEPS (iPEPS) corner transfer matrix (CTM) renormalization group (RG) techniques [42–45], making advantage of simplifications introduced by the use of point-group symmetric tensors [41]. At each RG step a truncation of the (Hermitian) CTM is done keeping (at most) $\chi$ eigenvalues and preserving exactly the $SU(2)$ multiplet structure. Energy optimization [46–48] is performed using a conjugate gradient (CG) method [49] up to a maximum $\chi = \chi_{\text{opt}}$ and then, eventually, one takes the limit $\chi \to \infty$ (using a “rigid” ansatz) by extrapolating the data [41].

We now turn to the results. In Fig. 2 we show the scaling of the iPEPS energies vs $D^2/\chi$ for the two local chiral Hamiltonians studied here, and different choices of the virtual space $V$ up to $D \leq 5$. Using linear fits, one obtains accurate variational energies in the $\chi \to \infty$ limit, apart from $D = 5$ for which the CTM RG converges to unphysical (pairs of) solutions beyond $\chi = 2D^2$. The exact GS energies obtained on a small periodic 30-site cluster [22] (expected to give a lower bound of the true thermodynamic values) provide a first reference, showing that the iPEPS energies are remarkably accurate. For the second model in Fig. 2(b), we have compared our results to the variational energy of the KL ansatz computed with Monte Carlo [22]. We find that, even for the smallest bond dimensions $D = 3$ ($V = \frac{1}{2} \oplus 0$) and $D = 4$ ($V = \frac{1}{2} \oplus 0 \oplus 0$), the iPEPS energy is lower than the energy of the KL CSL. This provides solid arguments that these chiral $SU(2)$-invariant PEPS are very good variational states. Hereafter we investigate further their edge and bulk properties and point out similarities and differences with the KL wave function.

Chiral edge modes. First, we have computed the entanglement spectrum (ES) of the optimized $D = 3$ PEPS on an infinitely-long cylinder $C$, bi-partitioned into two semi-infinite half-cylinders $C_L$ and $C_R$, $C = C_L \cup C_R$. This can be done exactly [50] on cylinders with up to $N_v = 8$ sites of circumference. Li and Haldane [51] have conjectured that, in chiral topological states, there is a deep one-to-one correspondence between the true physical edge spectrum and the ES [52, 53]. The ES is obtained from the leading eigenvector of the finite-dimensional $D^{2N_v} \times D^{2N_v}$ transfer matrix of the cylinder, as originally proposed in Ref. 50, and already applied to chiral spin liquids [38, 39]. The ES shown in Fig. 3 as a function of the momentum $K$ along the cut clearly reveal the existence of well-defined chiral branches linearly dispersing as $E_K \sim v K$. One also sees quasi-degenerate groups of levels whose counting (in terms of $SU(2)$ multiplets) matches exactly the one of the $SU(2)_1$ WZW CFT [13], as expected in a KL CSL phase [54]. Note that the ES of the optimized PEPS is remarkably similar to the one obtained for another studied chiral PEPS [38, 39], certainly belonging to the same $D = 3$ chiral PEPS family, but far away in parameter space. Although, the same exact calculation cannot be realized for $N_v = 8$ beyond $D = 3$, we conjecture that the $SU(2)_1$ chiral edge modes are genuine features of our chiral PEPS optimized for Hamiltonian (1).

**Bulk properties.** The KL CSL is expected to have short-range (spin-spin) correlations [16] as the bosonic $\nu = 1/2$ FQH state it derives from. We investigate now the correlation functions of the PEPS ansatz, and establish important differences. We use the same definitions and CTM RG procedure as described in the study of the frustrated AFHM and focus on the two cases $D = 3$ ($V = \frac{1}{2} \oplus 0$) and $D = 4$ ($V = \frac{1}{2} \oplus 0 \oplus 0$). Fig. 4(a) shows the spin-spin correlations vs distance on a semi-log plot. At short distance, we observe a rapid exponential fall-off characteristic of the KL CSL. However our data clearly show additional exponential tails with much larger characteristic length but with much smaller weight. In other words, we can parametrize the correlation function vs distance as

$$C_S(d) = \sum_{\xi_{\text{min}} \leq \xi \leq \xi_{\text{max}}} w(\xi) \exp(-d/\xi),$$

where the short distance decay is characterized by $w(\xi_{\text{min}}) \simeq 1$ while, at long distance, the slower decay $\exp(-d/\xi_{\text{max}})$ takes over with $\xi_{\text{max}} \gg \xi_{\text{min}}$ and $w(\xi_{\text{max}}) \ll 1$. In fact, we think that $\xi_{\text{max}} \to \infty$ when $\chi \to \infty$ (see Fig. 4(b)) while, simultaneously, $w(\xi_{\text{max}})$ goes very rapidly to zero. If, as suggested in Fig. 4(c), $w(\xi) \propto \exp(-\xi/\lambda)$, where $\lambda \simeq 0.7 \simeq \xi_{\text{min}}$, $C_S(d)$ will show a typical stretched exponential form at long distance, $C_S(d) \sim (d/\lambda)^\gamma \exp(-d/\lambda)^\gamma$. In any case,
C_S(d) should exhibit a “gossamer tail” which decays slower than any single exponential function.

The dimer-dimer correlations are shown in Fig. 5(a). The asymptotic long-distance behaviors can always be fitted as exponential decays. The correlation lengths extracted from the fits are found to diverge linearly with \( \chi \), for both model studied, as shown in Fig. 5(b). At short distance, the data are better fitted as a power law \( d^{-\alpha} \), although with a large exponent \( \alpha \approx 4.5 \), rather than as an exponential. Thus, the power-law behavior takes over at all distances when \( \chi \rightarrow \infty \). This suggests a form of emerging \( U(1) \)-gauge symmetry typical of dimer liquids [55] or RVB states [56–59] on bipartite lattices.

**Summary and outlook.** Using a previous symmetry classification of \( SU(2) \)-invariant PEPS we have constructed simple families of chiral PEPS on the square lattice. Using iPEPS supplement by a CG algorithm, we have optimized these PEPS w.r.t the local chiral (frustrated) AFHM, believed to host a CSL phase of the same form of emerging \( \chi \) takes over at all distances when \( \chi \) is larger than as an exponential. Thus, the power-law behavior takes over at all distances when \( \chi \rightarrow \infty \). This suggests a form of emerging \( U(1) \)-gauge symmetry typical of dimer liquids [55] or RVB states [56–59] on bipartite lattices.

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