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Establishing non-Abelian topological order in Gutzwiller-projected Chern insulators via entanglement entropy and modular $\mathcal{S}$-matrix

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We use entanglement entropy signatures to establish non-Abelian topological order in projected Chern-insulator wave functions. The simplest instance is obtained by Gutzwiller projecting a filled band with Chern number $C = 2$, whose wave function may also be viewed as the square of the Slater determinant of a band insulator. We demonstrate that this wave function is captured by the $SU(2)_2$ Chern-Simons theory coupled to fermions. This is established most persuasively by calculating the modular $\mathcal{S}$-matrix from the candidate ground-state wave functions, following a recent entanglement-entropy-based approach. This directly demonstrates the peculiar non-Abelian braiding statistics of Majorana fermion quasiparticles in this state. We also provide microscopic evidence for the field theoretic generalization, that the Nth power of a Chern number C Slater determinant realizes the topological order of the $SU(N)_C$ Chern-Simons theory coupled to fermions, by studying the $SU(2)_3$ (Read-Rezayi–type state) and the $SU(3)_2$ wave functions. An advantage of our projected Chern-insulator wave functions is the relative ease with which physical properties, such as entanglement entropy and modular $\mathcal{S}$-matrix, can be numerically calculated using Monte Carlo techniques.

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It is well known that quasiparticles may go beyond the conventional bosonic and fermionic statistics in two-dimensional many-body systems. A famous example is the Laughlin quantum Hall state that is realized by interacting electrons in fractionally filled Landau levels.[1] These are described by the Laughlin wave function,[2] where the quasiparticles carry fractional statistics. This state realizes an Abelian topological order,[3] described by a relatively well-understood[4] low-energy effective theory, the U(1) Chern-Simons (CS) theory.

There is increasing interest in generalizations to non-Abelian statistics, partially brought on by the recent preliminary evidence for Majorana fermions in superconductor-semiconductor junctions[5] and their potential as topological quantum memories.[6–8] Other examples of non-Abelian topological order are the $\nu = 5/2$ and $\nu = 12/5$ fractional quantum Hall effects[9] and the Moore-Read states.[10] Although a general theory and classification of these states are still absent, there is a wide class of states effectively characterized by non-Abelian CS theories:[11] the low-energy effective theory for filling fraction $\nu = k/N$ on k Landau levels is the $SU(N)_k$ CS theory. In the simplest case of $SU(2)_2$ CS theory, the elementary excitations are Ising anyons, whose braiding transforms the ground state, instead of just incurring phase factors corresponding to anionic statistics as in the Abelian case.[12] The entanglement spectrum has also been established as a powerful tool for identifying such phases in numerical calculations.[13] For universal quantum computation, the minimal $SU(2)_2$ non-Abelian statistics is insufficient. Instead, one needs at least the complexity of $SU(2)_3$ topological order with Fibonacci anyons,[8] which may describe the fractional quantum Hall plateau at $\nu = 12/5$. Examples of such phases are given by the Read-Rezayi states[14] and generalizations to lattice spin liquid states;[15,16] however, physical properties of these constructions are relatively difficult to evaluate.

Fractional quantum Hall liquids are generally associated with extreme experimental conditions such as clean samples and large magnetic fields. Yet it is increasingly being appreciated that Landau levels are not the sole route to realizing these states. It is well known that the integer quantum Hall effect is present in Chern insulators—lattice band models without an external magnetic field but with a net Berry curvature in reciprocal space.[17] Analogous interacting lattice models offer a new route to realizing topological orders, for which there has been mounting numerical evidence both for Abelian[18–22] and non-Abelian[23–26] states, which are collectively referred to as fractional Chern insulators.

Recall that the Laughlin wave functions[2] $\psi \sim \prod(z_i - z_j)^m e^{-|z_k|^2/4}$ can be considered as the mth power of a lowest-Landau-level integer quantum Hall state of anyons with a reduced charge. Previously, we confirmed that the lattice analog of this statement: the mth power of a Chern band wave function with unit Chern number $\psi \sim \psi^m_{C=1}$, has the topological order of a Laughlin state of order m.[27,28] In this paper, we focus on the cases when the Chern number $C > 1$, which is *unique* to lattice models and has no simple Landau-level counterpart. Consistent with the field theory study in Ref. 29 and parton construction scheme proposed in Ref. 30, we suggest that the square (power $N = 2$) of $C = 2$ Chern band wave functions $\psi \sim \psi^2_{C=2}$ are captured by the $SU(2)_2$ CS theory coupled to fermions and have the same quasiparticle braiding statistics as the Moore-Read Pfaffian state[31] $\psi \sim \mathrm{Pf}(\frac{1}{z_i - z_j})\prod(z_i - z_j)e^{-|z_k|^2/4}$. We verify that there are only three linearly independent wave functions by construction, consistent with the expected threefold ground-state degeneracy. Especially, the wave function diagnostic algorithm in Ref. 28 can be generalized to non-Abelian cases and is particularly useful for many-body systems where the entanglement spectrum is not available. With a variational ansatz, physical measurables of these states are much simpler to calculate, thus we are able to extract the modular $\mathcal{S}$-matrix easily and determine the quantum dimension and quasiparticle statistics through topological entanglement entropy (TEE)[27,28,32,33] and prove the existence of non-Abelian quasiparticles. This is a direct numerical measurement of the modular $\mathcal{S}$-matrix and identification of a non-Abelian topological-order wave function. We also generalize our studies of ground-state degeneracy and entanglement to the $C = 2$, $N = 3$ ($\psi \sim \psi_{C=2}^3$) and $C = 3$, $N = 2$ ($\psi \sim \psi_{C=3}^2$) cases. These results imply the effective theory for the Nth power of a $C = k$ Chern insulator's band $\psi \sim \psi_{C=k}^N$ is the $SU(N)_k$ CS theory coupled to fermions, allowing non-Abelian statistics when $N > 1$ and $k > 1$. Besides, these constructions may offer access to the entire ground-state manifold with different choices of boundary conditions of the parent Chern insulator.

Chern number $C = 2$ model. To construct a two-band model with Chern number $C = \pm 2$, consider a tight-binding model on a two-dimensional square lattice with two orbitals on each lattice site labeled by $I = 1,2$:

$$H = \sum_{\langle ij\rangle,I}(-1)^{I+1}c_{jI}^\dagger c_{iI} + \sum_{\langle ij\rangle}(e^{i2\theta_{ij}}c_{j2}^\dagger c_{i1} + \text{H.c.}) + \Delta\sum_{\langle\langle ik\rangle\rangle}(e^{i2\theta_{ik}}c_{k2}^\dagger c_{i1} + \text{H.c.}), \quad (1)$$

where θ_{ij} is the azimuthal angle for the vector connecting i and j. By counting the number of chiral modes on the physical edges as well as within the entanglement spectrum, we verify that the model has a finite gap between the two bands with Chern number $C = \pm 2$, respectively. Hereafter, we assume $\Delta = 1/\sqrt{2}$ for a maximum gap to suppress the finite-size effect. For a system at half filling with periodic boundary conditions, the many-body ground state occupies the valence band below the band gap, and the corresponding wave function $\chi(z_1,z_2,\dots)$ is a Slater determinant, where $z = (\vec{r},I)$ contains both the position and orbital indices.

Gutzwiller projected wave functions. Our wave functions' construction generalizes previous chiral spin liquid parton constructions,[27,34–36] but instead of occupying a band with Chern number $C = 1$, each parton now fills up a band with Chern number $C > 1$, e.g., the Hamiltonian in Eq. (1). It is then restricted to one fermion per site Hilbert space by Gutzwiller projection. For the simplest case with two flavors of partons labeled as spin up and spin down at half filling, the resulting wave function is $\Phi(z_1,z_2,\dots) = \chi_\uparrow(z_1,z_2,\dots)\chi_\downarrow(\tilde{z}_1,\tilde{z}_2,\dots)$, where $\tilde{z}_i$ are the set of complementary sites of z_i. Note that all the charge degrees of freedom are now projected out, $\Phi(z_1,z_2,\dots)$ is a spin wave function and is purely bosonic. In addition, Eq. (1) has a particle-hole symmetry $c_{\vec{r}I}^\dagger \leftrightarrow c_{\vec{r}I}(-1)^{r_x+r_y}$, which simplifies $\Phi(z_1,z_2,\dots) = \chi^2(z_1,z_2,\dots)$ up to an unimportant sign. The properties of $\chi^2(z_1,z_2,\dots)$ are the major focus of this paper. Note that it is $\pi/2$-rotational symmetric even though $\chi(z_1,z_2,\dots)$ is not; although the $\pi/2$ rotation symmetry is not essential to the topological properties, it is especially helpful for their determination.[28]

To construct $\chi^2(z_1,z_2,\dots)$ with periodic boundary conditions, there are multiple choices of boundary conditions for the parent Chern insulator, e.g., either periodic or antiperiodic boundary condition along the $\hat{x}$ and $\hat{y}$ directions in Eq. (1). Let us denote the four corresponding projected wave functions as $|\Phi_x\Phi_y\rangle$, $\Phi_{x,y} = 0,\pi$. Physical quantities related to the wave functions may be calculated with variational Monte Carlo method.[37] To understand their relation and linear dependence, we calculate the overlaps between them with variational Monte Carlo method on a 12×12 system:

$$\begin{aligned}\langle 00|\pi\pi\rangle &= \alpha,\\ \langle 0\pi|\pi 0\rangle &= \alpha',\\ \langle 0\pi|00\rangle &= \langle \pi 0|00\rangle = \beta,\\ \langle 0\pi|\pi\pi\rangle &= \langle \pi 0|\pi\pi\rangle = \beta'.\end{aligned} \quad (2)$$

Numerically, we find to very high accuracy that $\alpha = \alpha' = -0.086$ and $\beta = \beta' = 0.457$. We may construct a "generalized" projection operator:

$$P = \sum |\Phi_x\Phi_y\rangle\langle\Phi_x\Phi_y||\Phi_x'\Phi_y'\rangle\langle\Phi_x'\Phi_y'| = \begin{pmatrix}|\pi 0\rangle\\ |0\pi\rangle\\ |\pi\pi\rangle\\ |00\rangle\end{pmatrix}^T \begin{pmatrix}1 & \alpha & \beta & \beta\\ \alpha & 1 & \beta & \beta\\ \beta & \beta & 1 & \alpha\\ \beta & \beta & \alpha & 1\end{pmatrix} \begin{pmatrix}\langle\pi 0|\\ \langle 0\pi|\\ \langle\pi\pi|\\ \langle 00|\end{pmatrix}. \quad (3)$$

Due to the nonorthogonality between the basis states, the eigenvalues of P actually contain one 0, so the corresponding eigenstate is projected out:

$$P\,[|\pi\pi\rangle - |0\pi\rangle - |\pi 0\rangle + |00\rangle] = 0, \quad (4)$$

where we have used $2\beta = 1 + \alpha$ (true to high numerical accuracy). Thus there are only three linearly independent wave functions by construction:

$$\begin{aligned}|F_x = 1, F_y = 1\rangle &\simeq (|00\rangle + |0\pi\rangle + |\pi 0\rangle + |\pi\pi\rangle),\\ |F_x = 1, F_y = -1\rangle &\simeq (|00\rangle - |0\pi\rangle + |\pi 0\rangle - |\pi\pi\rangle),\\ |F_x = -1, F_y = 1\rangle &\simeq (|00\rangle + |0\pi\rangle - |\pi 0\rangle - |\pi\pi\rangle),\end{aligned} \quad (5)$$

up to phase and normalization. We have introduced the flux threading operators F_x and F_y to label these states. The wave functions' linear dependence is consistent with the ground-state degeneracy of $SU(2)_2$ CS theory, as shown in the Supplemental Material. These provide a complete basis for candidate ground-state wave functions, i.e., other possible constructions with different boundary conditions for partons are shown to be linearly dependent on the wave functions above.[38]

Topological entanglement entropy. To obtain further information on the wave functions, we extract their TEE for a 6×6 system following the prescription of Kitaev and Preskill,[32] which effectively cancels out the boundary and corner contributions and exposes the topological term, given the size of the regions exceed the correlation length. Although the smallest length scale is only two lattice spacings for the system size we study, it is still longer than the correlation length $\xi \sim 0.5$ lattice spacings. In addition, the corresponding wave-function overlaps suggest that the residue of Eq. (4) is just $\sim$1.3%; thus the orthogonal basis in Eq. (6) is still a good approximation. These facts suggest that the system size is large enough to reflect universal properties. Throughout we focus on the Renyi entropy S_2 due to its ease of calculation.[27,28,39]

We find that the TEE of $|\Phi_x\Phi_y\rangle$ for a topologically trivial disk-shape entanglement partition is $\gamma = 0.85 \pm 0.08$, in reasonable agreement with the ideal theoretical value $\lambda_{SU(2)_2} = \ln 2 \sim 0.693$ for the $SU(2)_2$ CS theory. Note that, for an Abelian topological order with $D^2 = 3$ degenerate ground states on a torus, the expected TEE would be

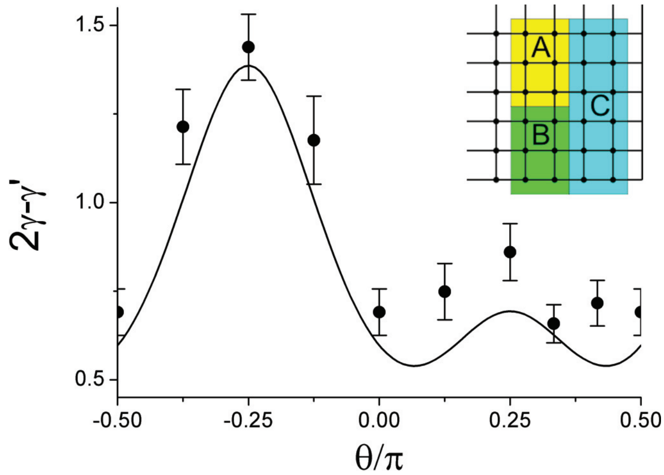


FIG. 1. (Color online) (Inset) Kitaev-Preskill scheme for extracting TEE by partitioning the torus into regions A, B, and C.[32] Regions C and AB encircle the torus, leading to a state-dependent TEE of γ', while the TEE γ for region A and B has a fixed value. The resulting $2\gamma - \gamma' = -S_{\rm ABC} + S_{\rm AB} + S_{\rm BC} + S_{\rm AC} - S_{\rm A} - S_{\rm B} - S_{\rm C} = -2S_{\rm A} + 2S_{\rm AB} - S_{\rm ABC}$ is plotted for the linear combinations of wave functions $|\Phi_1\rangle$. The solid curve is the theoretical value from the SU(2)$_2$ CS theory.

$\gamma = \ln D \sim 0.549$, which deviates further from the calculated value and is unlikely to describe these wave functions.

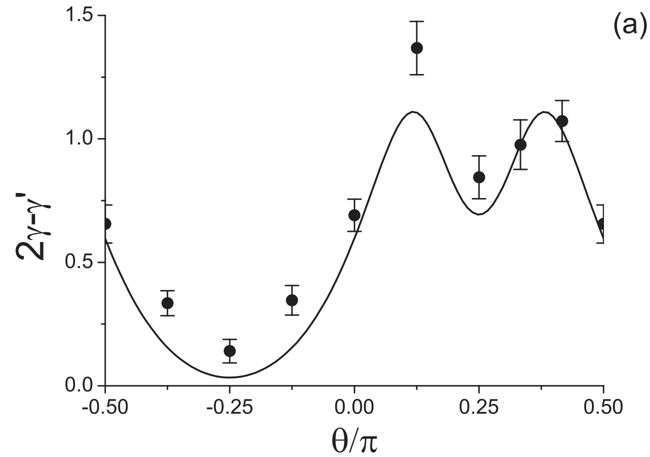
Modular $\mathcal{S}$-matrix from entanglement entropy. A decisive identification of the topological order is provided by extracting the braiding properties of quasiparticles using entanglement. Following the algorithm for a $\pi/2$-rotation symmetric system in Ref. 28, we (i) calculate the TEE γ' for partitioning the torus into two cylinders along the $\hat{y}$ direction for various linear combinations of wave functions (see Fig. 1 inset), then (ii) search for the states with minimum entanglement entropy (maximum TEE γ') and identify them as the $\hat{y}$ direction Wilson loop states of quasiparticles, and finally (iii) establish their transformation under $\pi/2$ rotation, which gives the modular $\mathcal{S}$-matrix. The numerical results of TEE are shown as $2\gamma - \gamma'$ for the following linear combinations: $|\Phi_1\rangle = \cos\theta|0\pi\rangle + \sin\theta|\pi 0\rangle$, $|\Phi_2\rangle = \sin\theta|00\rangle - \cos\theta|\pi 0\rangle$, and

$$|\Phi_3\rangle = (\sin\theta + 0.7915\cos\theta)|00\rangle - (\sin\theta + 0.4697\cos\theta)|\pi 0\rangle - 1.2623\cos\theta|0\pi\rangle \quad (6)$$

for selected values of θ shown in Figs. 1, 2(a), and 2(b), respectively. By identifying the minima of $2\gamma - \gamma'$, we obtain the three orthogonal quasiparticle states, given approximately as[28]

$$\begin{aligned} |\Xi_1\rangle &= -|\pi 0\rangle - |00\rangle, \\ |\Xi_2\rangle &= -|\pi 0\rangle + |00\rangle, \\ |\Xi_3\rangle &= 0.7915|00\rangle - 0.4697|\pi 0\rangle - 1.2623|0\pi\rangle. \end{aligned} \quad (7)$$

Now consider a rotation of $\pi/2$: the states $|\Phi_x\Phi_y\rangle$ transform as $|\pi 0\rangle \leftrightarrow |0\pi\rangle$ and $|00\rangle \leftrightarrow |00\rangle$, which determines the transformation of $|\Xi_j\rangle$. Along with Eq. (2) to ensure the orthogonality of wave functions, it leads to the following $\mathcal{S}$-matrix:



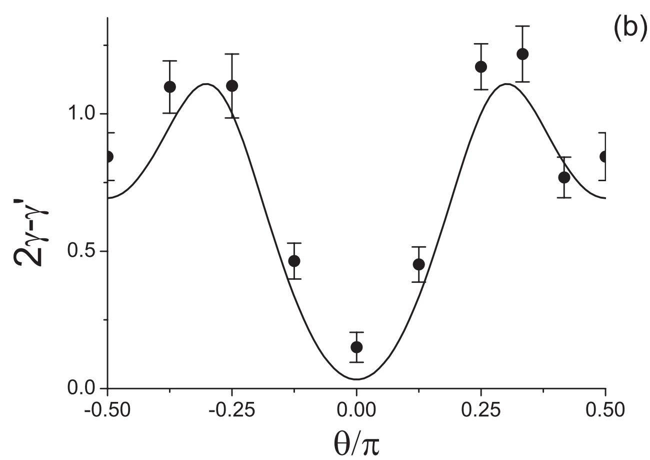


FIG. 2. TEE $2\gamma - \gamma'$ for linear combinations of wave functions: (a) $|\Phi_2\rangle$ and (b) $|\Phi_3\rangle$. The solid curves are the theoretical values from the SU(2)$_2$ CS theory. The presence of only two minima with $2\gamma - \gamma' \simeq 0$ indicates that two of the three quasiparticles are Abelian, while the third one must be non-Abelian.

$$\mathcal{S} = \begin{pmatrix} 0.627 & 0.610 & 0.484 \\ 0.610 & 0.000 & -0.792 \\ 0.484 & -0.792 & 0.372 \end{pmatrix}. \quad (8)$$

As a comparison, the ideal $\mathcal{S}$-matrix for the SU(2)$_2$ CS theory is

$$\mathcal{S} = \begin{pmatrix} 0.5 & 0.707 & 0.5 \\ 0.707 & 0 & -0.707 \\ 0.5 & -0.707 & 0.5 \end{pmatrix}. \quad (9)$$

While there is a reasonably quantitative agreement, what is more revealing are the robust qualitative features of quasiparticle braiding that the obtained $\mathcal{S}$-matrix Eq. (8) implies. While the quasiparticles corresponding to $|\Xi_1\rangle$ and $|\Xi_3\rangle$ obey Abelian statistics upon braiding, the zero diagonal entry in the modular $\mathcal{S}$-matrix for the quasiparticle of $|\Xi_2\rangle$ is a signature of its non-Abelian self-statistics. Indeed, for the Majorana fermion in the SU(2)$_2$ CS theory, one Dirac fermion composes a pair of Majorana fermions $c = \gamma_1 + i\gamma_2$; when one of the Majorana fermions braids with another Majorana fermion and picks up an additional π phase, it changes the original annihilation operator to a creation operator and vice versa and fails to return to the excitation-free ground state, thus the corresponding entry in the modular $\mathcal{S}$-matrix vanishes.

We make two more detailed comparisons between numerics on these wave functions and the $SU(2)_2$ CS theory, which predicts the following connection between the eigenstates of F_x and F_y in Eq. (6) and the quasiparticles:[12]

$$\begin{aligned} |F_x = 1, F_y = 1\rangle &= (|1_y\rangle + |\psi_y\rangle)/\sqrt{2}, \\ |F_x = 1, F_y = -1\rangle &= (|1_y\rangle - |\psi_y\rangle)/\sqrt{2}, \\ |F_x = -1, F_y = 1\rangle &= |\sigma_y\rangle, \end{aligned} \tag{10}$$

where $|1_y\rangle$, $|\psi_y\rangle$, and $|\sigma_y\rangle$ are the $\hat{y}$ direction Wilson loop states of the identity, fermionic, and non-Abelian quasiparticles, respectively. The connection between Eqs. (6) and (10) gives the expressions of the $|\Phi_x\Phi_y\rangle$ states in the $|1_y\rangle$, $|\psi_y\rangle$, $|\sigma_y\rangle$ basis:

$$\begin{aligned} |00\rangle &= 0.8466|1_y\rangle + 0.1101|\psi_y\rangle + 0.5208|\sigma_y\rangle, \\ |\pi 0\rangle &= 0.8466|1_y\rangle + 0.1101|\psi_y\rangle - 0.5208|\sigma_y\rangle, \\ |0\pi\rangle &= 0.1101|1_y\rangle + 0.8466|\psi_y\rangle + 0.5208|\sigma_y\rangle, \\ |\pi\pi\rangle &= 0.1101|1_y\rangle + 0.8466|\psi_y\rangle - 0.5208|\sigma_y\rangle, \end{aligned} \tag{11}$$

consistent with Eq. (7). In addition, for an arbitrary ground state, the value of TEE is given by[40]

$$2\gamma - \gamma' = -\ln\left(\sum_j p_j^2/d_j^2\right), \tag{12}$$

where d_j and p_j are the individual quantum dimension and the statistical weight for the jth quasiparticle. We may derive d_j from the values of the $2\gamma - \gamma'$ minima as $\ln(d_j^2) = 2\gamma - \gamma_j'$, which follows straightforwardly from Eq. (12), and we obtain $d_1 = d_\psi = 1$, $d_\sigma = \sqrt{2}$. The values of $2\gamma - \gamma'(\theta)$ with these individual quantum dimensions and Eq. (11) are shown in Figs. 1 and 2 as the solid curves and fit well with the numerical results. In particular, $d_\sigma = \sqrt{2}$ implies that the σ quasiparticle must obey non-Abelian statistics.

Other non-Abelian states (i) SU$(3)_2$. Such wave-function constructions may be generalized to even more complicated non-Abelian cases. As another example, we construct nine candidate ground-state wave functions $|\Phi_x\Phi_y\rangle$ with boundary conditions $\Phi_{x,y} = 0, \pm 2\pi/3$ for $\chi^3(z_1, z_2, \ldots)$, the cube of the Chern-insulator wave functions. Repeating the calculations and analysis in previous sections on a 12×12 system, we obtain a "generalized" projection operator P' (see Ref. 41), which has only six nonzero eigenvalues; therefore, there are only six linearly independent wave functions by construction. The $\pi/2$-rotation eigenvalues of the six corresponding eigenstates are ± 1, ± 1, and $\pm i$. These results are consistent with $SU(3)_2$ CS theory. In addition, the TEE for a contractible entanglement partition on a 6×6 system is $\gamma \simeq 1.264 \pm 0.073$, consistent with the theoretical value of $D = [3(5+\sqrt{5})/2]^{1/2}$ and $\gamma_{SU(3)_2} = \ln D \simeq 1.19$. While we consider this evidence sufficient, we leave further verifications such as TEE ground-state dependence and constructions from other boundary conditions to future works.

(ii) SU$(2)_3$ in close connection to the Read-Rezayi state. In analogy with Eq. (1), we may construct a triangular lattice tight-binding model with the azimuthal angular dependence 3θ. The model is a two-band Chern insulator with Chern number $C = \pm 3$ for $\Delta \neq 0$. Similar models may have potential for the construction of bands with even higher Chern number, and a systematic scheme to produce arbitrary Chern-number bands has been studied in Ref. 26. We construct wave functions with nine different boundary conditions on a 12×12 system. Our results show that only four of the nine eigenvalues of the corresponding "generalized" projection operator are unambiguously finite, consistent with the fourfold ground-state degeneracy of the $SU(2)_3$ CS theory.

In conclusion we have introduced lattice wave-function constructions for a class of non-Abelian topological phases that (i) are readily generalized to capture $SU(N)_k$ topological order, (ii) easily generate the set of candidate ground-state wave functions corresponding to the topological degeneracy. and (iii) can compute physical properties with Monte Carlo techniques, and the usefulness of entanglement in the diagnosis and study of these wave functions. The presence of such natural lattice wave functions holds promise that such states may be realized in the context of fractional Chern insulators.

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[31] Strictly speaking this wave function is not the same topological order as the Moore-Read Pfaffian state captured by the pure $SU(2)_2$ CS theory; although it shares the same ground-state degeneracy and quasiparticle excitation braiding encoded in the modular $\mathcal{S}$-matrix with the Pfaffian state, it differs at the level of the quasiparticle spin encoded in the modular T matrix due to the fermionic core for certain quasiparticles. Similar difference exists between the $SU(2)_k$ states we study and the Read-Rezayi states. See Ref. 41 for a detailed discussion. We do not focus on such distinctions because these states behave identical for the properties we study.

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