Projected Entangled-Pair States Can Describe Chiral Topological States

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We show that projected entangled-pair states (PEPS) in two spatial dimensions can describe chiral topological states by explicitly constructing a family of such states with a nontrivial Chern number. They are ground states of two different kinds of free-fermion Hamiltonians: (i) local and gapless; (ii) gapped, but with hopping amplitudes that decay according to a power law. We derive general conditions on topological free-fermionic projected entangled-pair states that show that they cannot correspond to exact ground states of gapped, local parent Hamiltonians and provide numerical evidence demonstrating that they can nevertheless approximate well the physical properties of topological insulators with local Hamiltonians at arbitrary temperatures.

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Introduction.—Projected entangled-pair states (PEPS) [\[1\]](#page-4-0) are believed to provide an accurate description of many-body quantum systems with local interactions in thermal equilibrium [[2](#page-4-1)]. At zero temperature, PEPS contain the necessary entanglement demanded by the area law in order to describe gapped Hamiltonians with local (shortrange) interactions [[3\]](#page-4-2). In fact, matrix-product states, the one-dimensional (1D) version of PEPS, have been a key tool leading to the classification of all possible phases of spin Hamiltonians of that kind [\[4](#page-4-3)–[6\]](#page-4-4). Furthermore, wellknown topological states in two dimensions (2D), such as the toric code [[7](#page-4-5)], resonating valence bond [\[8\]](#page-4-6), or string nets [[9](#page-4-7)], possess a simple and exact description within that family [[10](#page-4-8)[–13\]](#page-4-9). This seems to indicate that PEPS can also help us to characterize and classify the gapped (topological) phases in dimensions higher than one.

Despite the above indications, there exists a deep reason to believe that PEPS cannot describe the physics of certain kinds of topological phases, namely, those that have chirality. In fact, despite a significant effort in the research of tensor network states, we do not know any PEPS corresponding to a 2D chiral topological phase, not even for the simplest topological insulators [[14](#page-4-10),[16](#page-4-11)]. Those are freefermionic systems with a nontrivial Chern number $C \neq 0$ that can be thought of as the lattice counterpart of integer quantum Hall materials. This fact may be qualitatively understood as follows. Any PEPS is the ground state of a local so-called *parent* Hamiltonian $H = \sum_i h_i$ [[17](#page-4-12),[18](#page-4-13)]. This Hamiltonian is frustration free, meaning that the PFPS is Hamiltonian is frustration free, meaning that the PEPS is annihilated by each local term h_i individually. But if H corresponds to a free-fermion system with a gapped band structure, the Hamiltonian terms are of the form $h_i = b_i^{\dagger} b_i$,
where the *h*, are quasiparticle operators supported in a where the b_i are quasiparticle operators supported in a small region. Their Wannier functions must thus be localized, which in turn has been proven to be impossible for systems with a nontrivial Chern number [\[19](#page-4-14)[,20\]](#page-4-15). Still, the question whether PEPS can describe chiral topological insulators is open: first, even though their parent Hamiltonians would be gapless, they might still be ground states of other non-frustration-free gapped Hamiltonians (with nonlocalized Wannier functions); second, although they do not provide exact descriptions of all chiral states, they may still be able to approximate them accurately.

In this Letter, we explicitly construct a simple family of PEPS with Chern number $C \neq 0$ on a square lattice. Our construction is based on Gaussian fermionic PEPS (GFPEPS) [\[21\]](#page-4-16); that is, those that can be created out of the vacuum by applying a Gaussian function of creation and annihilation operators. By simple, we mean with the smallest possible bond dimension, i.e., where there are just four auxiliary fermions on each lattice site. This family of GFPEPS possesses correlation functions with a power-law decay as well as nonlocalized Wannier functions. In fact, they are the unique ground states of free-fermion, gapped Hamiltonians with hopping amplitudes following the same decay. Apart from that, as all PEPS, they are ground states of local parent Hamiltonians, which however, must be gapless due to the presence of critical correlations. Indeed, we prove that there cannot be GFPEPS with a nontrivial Chern number that have a finite-range and gapped parent Hamiltonian, since all such Hamiltonians are in the trivial phase. This result, however, does not rule out the possibility of using PEPS to approximate the ground state of a chiral topological insulator with a local Hamiltonian. In fact, we investigate this issue and conclude that this is possible, since the approximation improves exponentially in the number of fermionic modes in the bond. Finally, we show that by using mixed GFPEPS we can approximate the finite temperature properties of such systems as well.

Gaussian fermionic PEPS.—We start with an $N \times N$
ware lattice with periodic boundaries and f *physical* square lattice with periodic boundaries and f physical fermionic orbitals at each site, with creation (annihilation) operators $a_{\mathbf{r},j}^{\dagger}(a_{\mathbf{r},j})$, with $\mathbf{r}=(x, y)$ the site and $j=1,\ldots,f$

FIG. 1 (color online). Schematic of a GFPEPS in two dimensions. The Majorana modes (small gray balls) form virtual bonds indicated by blue lines, which are mapped to the physical fermions (red balls) by a Gaussian map denoted by big blue circles.

the orbital index; we will mostly work in the basis of physical Majorana operators $c_{\mathbf{r},2j-1} = a_{\mathbf{r},j}^{\dagger} + a_{\mathbf{r},j}$ and $c_{\mathbf{r},2j} = (-i)(a_{\mathbf{r},j}^{\dagger} - a_{\mathbf{r},j})$. To obtain a PEPS description of the system, we start out with maximally entangled virtual Majorana modes $\gamma_{\mathbf{r},\alpha}^v$ (with $\alpha = 1, ..., \chi$ and $v = l, r, u, d$) which are obtained by acting with $1 + i\gamma^r \gamma^l$ d), which are obtained by acting with $1 + i\gamma_{\mathbf{r},\alpha}^r \gamma_{(\mathbf{r}+(1,0)),\alpha}^l$ and $1 + i\gamma_{\mathbf{r},\alpha}^u \gamma_{(\mathbf{r}+(0,1)),\alpha}^d$ $1 + i\gamma_{\mathbf{r},\alpha}^u \gamma_{(\mathbf{r}+(0,1)),\alpha}^d$ $1 + i\gamma_{\mathbf{r},\alpha}^u \gamma_{(\mathbf{r}+(0,1)),\alpha}^d$ on the vacuum (see Fig. 1), yielding a pure state ρ_{in} [\[21\]](#page-4-16). Here, the number of Majorana bonds χ is a parameter that can be used to systematically enlarge the class of states. Subsequently, we apply the same linear map $\mathcal E$ to each lattice site **r**, which maps the 4χ auxiliary modes $\gamma_{\mathbf{r},\alpha}^{v}$ to the 2f physical modes $c_{\mathbf{r},s}$ ($s = 1,..., 2f$); this vields the translationally invariant fermionic PFPS ρ yields the translationally invariant fermionic PEPS ρ_{out} .

We now restrict to the case where the map $\mathcal E$ is Gaussian. Then, ρ_{out} is a free-fermion state, which can be described in terms of its *covariance matrix* (CM) Γ_{out} , defined as $(\Gamma_{\text{out}})_{(\mathbf{r},s),(\mathbf{r}',t)} = (i/2) \text{tr}(\rho_{\text{out}}[\epsilon_{\mathbf{r},s}, \epsilon_{\mathbf{r}',t}])$; similarly, for ρ_{in} we have $(\Gamma_{\text{in}})^{v,v'}_{(\mathbf{r},\alpha)}$ $\psi_{(\mathbf{r},\alpha),(\mathbf{r}',\beta)}^{v,v'} = (i/2) \text{tr}(\rho_{\text{in}}[\gamma_{\mathbf{r},\alpha}^v, \gamma_{\mathbf{r}',\beta}^{v'}])$. Finally, $\mathcal E$ can be expressed using a CM M defined on the $2f$ + 4χ modes $\{ (c_{\mathbf{r},s}), (\gamma_{\mathbf{r},\alpha}^v) \}$, which encodes how $\mathcal E$ correlates the input modes with the output modes [22] (an explicit the input modes with the output modes [\[22\]](#page-4-17) (an explicit expression will be given soon). These CMs are real, antisymmetric, and fulfill $\Gamma \Gamma^{\top} \leq \mathbb{I}$, where equality only holds for pure states (and purity-preserving maps).

Since we consider a translational invariant system of free fermions, it is most convenient to work in Fourier space. The Fourier transformed CM G_{in} of ρ_{in} , expressed in terms of Fourier transformed Majorana modes $\hat{\gamma}^v_{\mathbf{k},\alpha} = (1/N) \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} \gamma^v_{\mathbf{r},\alpha}$ [**k** = $(k_x, k_y), k_{x(y)}/(2\pi/N)$ = $0, \ldots, N - 1$, then reads

$$
G_{\rm in}(\mathbf{k}) = \begin{pmatrix} 0 & e^{ik_x} \mathbb{I}_{\chi} \\ -e^{-ik_x} \mathbb{I}_{\chi} & 0 \end{pmatrix} \oplus \begin{pmatrix} 0 & e^{ik_y} \mathbb{I}_{\chi} \\ -e^{-ik_y} \mathbb{I}_{\chi} & 0 \end{pmatrix}, \qquad (1)
$$

where \mathbb{I}_{χ} denotes a $\chi \times \chi$ identity matrix; the ordering of the modes is $\chi \times \chi$ d. The CM M for the Gaussian man \mathcal{E} the modes is l, r, u, d. The CM M for the Gaussian map $\mathcal E$ has a block structure

$$
M = \begin{pmatrix} A & B \\ -B^{\top} & D \end{pmatrix} = -M^{\top}, \tag{2}
$$

where $A \in \mathbb{R}^{2f \times 2f}$, $B \in \mathbb{R}^{2f \times 4\chi}$, and $D \in \mathbb{R}^{4\chi \times 4\chi}$ are variational parameters corresponding to physical and virtual iational parameters corresponding to physical and virtual modes. Any M with $MM^{\top} \leq \mathbb{I}$ characterizes an admissible $\mathcal E$. Applying $\mathcal E$ to the input ρ_{in} results in a CM [[22](#page-4-17),[23](#page-4-18)]

$$
G_{\text{out}}(\mathbf{k}) = B[D - G_{\text{in}}(\mathbf{k})]^{-1}B^{\top} + A \tag{3}
$$

expressed in terms of the Fourier transformed physical Majorana modes $d_{k,s} = (1/N) \sum_{\mathbf{r}} e^{-i\mathbf{k} \cdot \mathbf{r}} c_{\mathbf{r},s}$; G_{out} is pure if $MM^{\mathsf{T}} = \mathbb{I}$ (i.e. \mathcal{E} preserves purity). Expressing the if $MM^{\top} = \mathbb{I}$ (i.e., \mathcal{E} preserves purity). Expressing the inverse in Eq. ([3](#page-1-1)) by the adjugate matrix, one finds that $[G_{\text{out}}(\mathbf{k})]_{st} = [p_{st}(\mathbf{k})/q(\mathbf{k})]$, where $p_{st}(\mathbf{k})$ and $q(\mathbf{k}) =$ $det[D - G_{in}(\mathbf{k})]$ are trigonometric polynomials of degree $\leq 2\chi$ (Supplemental Material [[23](#page-4-18)]).

For pure GFPEPS, the class of quadratic Hamiltonians

$$
H_f = -i \sum_{\mathbf{k}} \sum_{s,t} \varepsilon(\mathbf{k}) [G_{\text{out}}(\mathbf{k})]_{st} d_{\mathbf{k},s} d_{\mathbf{k},t}^{\dagger} \tag{4}
$$

with spectrum $\varepsilon(\mathbf{k}) = \varepsilon(-\mathbf{k}) \ge 0$ has ρ_{out} as its ground state. These ''parent Hamiltonians'' can have different properties: (i) If $q(\mathbf{k}) > 0$, then for $\varepsilon(\mathbf{k}) \equiv 1$, H_f has exponentially decaying two-body interactions in real space, and by choosing $\varepsilon(\mathbf{k}) = q(\mathbf{k})$, one obtains a strictly local gapped Hamiltonian; (ii) if $q(\mathbf{k}) = 0$ for some **k** and $G_{out}(\mathbf{k})$ is continuous, $\varepsilon(\mathbf{k}) \equiv 1$ still yields a gapped Hamiltonian. Then, whether H_f has exponentially decaying terms depends on whether $G_{out}(\mathbf{k})$ has any discontinuities in its derivatives (which give rise to algebraically decaying terms in real space after Fourier transforming).

Example of a chiral GFPEPS.—Using this construction, we have obtained a family of chiral topological insulators whose ground states are GFPEPS. They have $f = 2$, $\chi =$ [2](#page-1-2), and M [Eq. (2)] is given by

$$
A = (-1 + 2\lambda) \begin{pmatrix} \omega & 0 \\ 0 & -\omega \end{pmatrix},
$$

\n
$$
B = \sqrt{\frac{\lambda - \lambda^2}{2}} \begin{pmatrix} \mathbb{I} - \omega & \mathbb{I} + \omega & -\sqrt{2}\omega & \sqrt{2}\mathbb{I} \\ \mathbb{I} - \omega & -\mathbb{I} - \omega & \sqrt{2}\mathbb{I} & -\sqrt{2}\omega \end{pmatrix},
$$

\n
$$
D = \begin{pmatrix} 0 & (-1 + \lambda)\mathbb{I} & -\frac{\lambda}{\sqrt{2}}\mathbb{I} & \frac{\lambda}{\sqrt{2}}\mathbb{I} \\ (1 - \lambda)\mathbb{I} & 0 & -\frac{\lambda}{\sqrt{2}}\mathbb{I} & -\frac{\lambda}{\sqrt{2}}\mathbb{I} \\ \frac{\lambda}{\sqrt{2}}\mathbb{I} & \frac{\lambda}{\sqrt{2}} & 0 & (-1 + \lambda)\mathbb{I} \\ -\frac{\lambda}{\sqrt{2}}\mathbb{I} & \frac{\lambda}{\sqrt{2}}\mathbb{I} & (1 - \lambda)\mathbb{I} & 0 \end{pmatrix},
$$

\n(5)

where

$$
\mathbb{I} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \text{ and } \omega = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}.
$$

The ordering of the physical Majorana modes is $(c_{11}, c_{21},$ c_{11} , c_{21}) and that of the virtual modes as in Eq. [\(1](#page-1-3)); here, $0 < \lambda < 1$. Using Eq. ([3](#page-1-1)), one finds that

FIG. 2 (color online). Correlation functions as given by $\left\| \left[\Gamma_{\text{out}}(\mathbf{r} - \mathbf{r}') \right] \right\|_{\text{tr}}$ for $\lambda = 1/\sqrt{2}$ on a 500 × 500 lattice as a function of the distance $\left| \mathbf{r} - \mathbf{r}' \right|$ along the x and y directions function of the distance $|\mathbf{r} - \mathbf{r}'|$ along the x and y directions
(blue crosses, both lie on top of each other) and along $\hat{x} + \hat{y}$ (blue crosses, both lie on top of each other) and along $\hat{x} + \hat{y}$ (green stars). Inset: Energy separation between the occupied and the unoccupied band as a function of k.

$$
G_{\text{out}}(\mathbf{k}) = \frac{1}{\tilde{q}(\mathbf{k})} \left(\int_{i[p_3(\mathbf{k})} p_1(\mathbf{k}) \omega \, d\mathbf{k} \right) \left[p_3(\mathbf{k}) \mathbb{I} - p_2(\mathbf{k}) \omega \right] \right)
$$

with $p_1(\mathbf{k}) = -2(1 + \cos k_x)(1 + \cos k_y)(1 - 2\lambda) - \lambda^2 \times$
 $[1 + 2\cos k_x + \cos k_y (2 + 3\cos k_y)]$ $p_1(\mathbf{k}) = 2(-\lambda + \lambda^2) \times$ $[1+2\cos k_y + \cos k_x(2+3\cos k_y)], p_2(\mathbf{k}) = 2(-\lambda + \lambda^2)\times$
(1+cosk)sink $p_2(\mathbf{k}) = 2(\lambda - \lambda^2)(1+\cos k) \sin k$ and $(1+\cos k_y)\sin k_x$, $p_3(\mathbf{k})=2(\lambda-\lambda^2)(1+\cos k_x)\sin k_y$, and $\tilde{q}(\mathbf{k}) = 2(1 + \cos k_x)(1 + \cos k_y)(1 - 2\lambda) + \lambda^2[3 + 2\cos k_y +$ $\cos k_x(2+\cos k_y)$; note that $G_{\text{out}}(\mathbf{k})$ is continuous but nonanalytic at $\mathbf{k} = (\pi, \pi)$.

Employing Eq. [\(4](#page-1-4)), we can now define particle-numberconserving parent Hamiltonians for G_{out} : If we choose $\varepsilon(\mathbf{k}) \equiv 1$, we obtain a gapped flat-band Hamiltonian with algebraically decaying hoppings (see Fig. [2\)](#page-2-0), whereas if we choose $\epsilon(\mathbf{k}) = q(\mathbf{k})$, we obtain a strictly local Hamiltonian with only next-nearest neighbor couplings, which however, is gapless at $\mathbf{k} = (\pi, \pi)$ (inset of Fig. [2\)](#page-2-0). In the first case, the Chern number can be computed from G_{out} (Supplemental Material [\[23](#page-4-18)]) and is found to be $C = -1$ for all $0 < \lambda < 1$. Note that by changing to the basis $c_{1\uparrow} \pm c_{2\downarrow}, c_{2\uparrow} \pm c_{1\downarrow}, G_{\text{out}}$ decouples into two GFPEPS describing spinless topological superconductors, each with $\chi = 1$ and equal chiralities.

Conditions for topological GFPEPS.—Let us now show that topological GFPEPS are very special. In particular, we will prove that any GFPEPS with a property known as injectivity [\[24\]](#page-4-19) (which holds generically), or more generally for which $q(\mathbf{k})$ is nonsingular, has a gapped local parent Hamiltonian that is connected to a trivial state via a gapped path and therefore cannot be topological; this implies that the parent Hamiltonians defined via $\epsilon(\mathbf{k}) =$ $q(\mathbf{k})$ have to be gapless. (This shows that injectivity in GFPEPS is much stronger than for general PEPS, where it does not have implications about the spectrum or the phase except for 1D systems.)

Let us first define injectivity for GFPEPS: By blocking $n_v \times n_h$ sites to a new supersite (by tracing over the virtual
particles), we can reach a point where the number of particles), we can reach a point where the number of physical Majorana modes $d_{ph} = 2f n_h n_v$ is larger than the number of virtual modes $d_{\text{vir}} = 2\chi(n_h + n_v)$. Then, $G_{\text{out}}(k) = B_{\Box}[D_{\Box} - G_{\text{in}}(k)]^{-1}B_{\Box}^{\top} + A_{\Box}$, where \Box denotes the corresponding matrices after blocking. We say that a GFPEPS is injective if there is a finite blocking size such that rank $(B_{\Box}) = d_{\text{vir}}$; i.e., the virtual system $G_{\text{in}}(\mathbf{k})$ is fully mapped onto the physical space. In this case, we can use a singular value decomposition of B_{\Box} = $\mathbb{V}^T \Sigma U$, where \mathbb{V} is an isometry, $\mathbb{V}^T = \mathbb{I}_{d_{\text{vir}}}$, and Σ is a diagonal strictly positive matrix to obtain from Eq. (3) diagonal strictly positive matrix, to obtain from Eq. [\(3\)](#page-1-1) $\mathbb{V}(\widetilde{G}_{\text{out}}(\mathbf{k}) - \widetilde{A}_{\Box}) \mathbb{V}^{\top} = \Sigma U[D_{\Box} - G_{\text{in}}(\mathbf{k})]^{-1} U^{\top} \Sigma,$
which implies which implies

$$
\det[\mathbb{V}(G_{\text{out}}(k) - A_{\Box})\mathbb{V}^{\top}] = \frac{\det^2(\Sigma)}{\det[D_{\Box} - G_{\text{in}}(k)]}.
$$
 (6)

Since all terms on the left-hand side are entries of CMs and thus bounded, it follows that $q_{\Box}(\mathbf{k}) :=$ $\det[D_{\Box} - G_{\rm in}(\mathbf{k})] \ge \delta > 0$ [in particular, the parent Hamiltonian of the blocked GFPEPS with $\varepsilon(\mathbf{k}) = q_{\Box}(\mathbf{k})$ in Eq. ([4](#page-1-4)) is gapped and local].

It is now exactly this property that allows us to construct a gapped interpolation from $G_{\text{out}}(k)$ to the topologically trivial state by adiabatically disentangling pairs of Majorana bonds (we can take n_v , n_h to be even, since injectivity is stable under blocking) via

$$
\Gamma_{\text{in}}^{\varphi} = \begin{pmatrix} \omega \sin \varphi & \cos \varphi \\ -\mathbb{I} \cos \varphi & \omega \sin \varphi \end{pmatrix} . \tag{7}
$$

Here, $\Gamma_{\text{in}}^{\varphi}$ is the CM of pairs of Majorana bonds on horizontally or vertically adjacent sites, which for $\varphi = 0$ describes a maximally entangled state, corresponding to the initial GFPEPS, whereas $\overline{\Gamma}_{in}^{\pi/2}$ corresponds to a product state, and thus, $G_{\text{out}}^{\pi/2}$ describes a topologically trivial state [\[25\]](#page-4-20). Since from Eq. [\(6](#page-2-1)), $det[D_{\square} - G_{\text{in}}^{\varphi}(k)] > 0$ for all $\varphi \in [0, \pi/2]$ this internalation corresponds to a smooth $\varphi \in [0, \pi/2]$, this interpolation corresponds to a smooth gapped local Hamiltonian, showing that any injective GFPEPS is in the trivial phase.

This argument can be generalized to the case where rank $(B_{\square}) < d_{\text{vir}}$ (i.e., the state is noninjective), as long as $d_{\text{vir}} \leq d_{\text{ph}}$ and $q_{\square}(\mathbf{k}) = \det[D_{\square} - G_{\text{in}}(\mathbf{k})] > 0$. In this case, define $\Delta := \min_{\mathbf{k}} \det[D_{\Box} - G_{\text{in}}(\mathbf{k})]$. It is always
possible to rotate M_{\Box} into $M'_{\Box} = e^{-\epsilon Z} M_{\Box} e^{\epsilon Z}$ with some
appropriate $Z = -Z^{\top}$ to obtain $\text{rank}(B_{\Box}) = d_{\Box}$ while appropriate $Z = -Z^{\overline{1}}$ to obtain rank $(B_{\square}) = d_{\text{vir}}$, while keeping det $[D'_0 - G_{in} (k)] > 0$ if ϵ is sufficiently
small compared to Λ . From there it is again possible to small compared to Δ . From there, it is again possible to perform an adiabatic evolution to the trivial state as before. If the initial GFPEPS was particle-number conserving, this symmetry can be kept along the path by using a particle-number-conserving interpolation $\Gamma_{\text{in}}^{\varphi}$. Thus, our

FIG. 3 (color online). (a) Error δ (see text) of the covariance matrix for $T = 0$, $e_S = 1$ (blue circles), entropy S_{GFPEPS} of the optimized GFPEPS (red crosses), difference between the Hall conductivity $-(\sigma_{xy}/2\pi)$ and the Chern number $C = -1$ (green
stars) for the optimized GEDEPS as a function of the number of stars) for the optimized GFPEPS as a function of the number of Majorana modes χ . (b) The blue dashed curve and solid green curve denote the Hall conductivity of the exact thermal state and GFPEPS, respectively, as a function of the von Neumann entropy of the exact state S_{ex}/N^2 . (c) Relative error of the free energy per site of the optimized GFPEPS as a function of S_{ex}/N^2 . The entropies of the optimized GFPEPSs were roughly proportional to S_{ex} . The Chern numbers of the Hamiltonians of which they are thermal states were always $C = -1$. (d) Relative error of the free energy per site of the optimized GFPEPS as a function of the parameter e_s of the exact state at $T = 0$. The optimized GFPEPSs with Chern number $C = 0$ are displayed by green crosses and those with $C = -1$ by open blue circles.

proof applies to both topological insulators and topological superconductors.

Numerical results.—We have performed numerical calculations on a 10×10 lattice for the model
 $H = \sum (a^{\dagger} a^{\dagger}) (\sigma \cdot d(k)) (a \cdot a \cdot \mu)^{\dagger}$ with $\sigma =$ $H = \sum_{\mathbf{k}} (a_{\mathbf{k},\uparrow}^{\dagger}, a_{\mathbf{k},\downarrow}^{\dagger}) (\boldsymbol{\sigma} \cdot \mathbf{d}(\mathbf{k})) (a_{\mathbf{k},\uparrow}, a_{\mathbf{k},\downarrow})$ $H = \sum_{\mathbf{k}} (a_{\mathbf{k},\uparrow}, a_{\mathbf{k},\downarrow}) (\boldsymbol{\sigma} \cdot \mathbf{d}(\mathbf{k})) (a_{\mathbf{k},\uparrow}, a_{\mathbf{k},\downarrow})$, with $\boldsymbol{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ the Pauli matrices and $\mathbf{d}(\mathbf{k}) = (\sin k_1 - \sin k_2) - \cos k_2 - \cos k_3$. with $\boldsymbol{\sigma}$ =
and $\boldsymbol{d}(\boldsymbol{k})$ = $(\sin k_v, -\sin k_x, 2 - \cos k_x - \cos k_y - e_s)$. This model has Chern number $C = -1$ for $0 < e_S < 2$, $C = 1$ for $2 <$ $e_S < 4$, and $C = 0$ otherwise [\[27\]](#page-4-21).

First, we determined the minimal distance $\delta :=$ $\max_{\mathbf{k}}||G_{\text{ex}}(\beta, \mathbf{k}) - G_{\text{GFPEPS}}(\mathbf{k})||_{\text{tr}}$ between the CM of $e^{-\beta H}/tr(e^{-\beta H})$ (for $e_S = 1$) at $\beta = \infty$ and the one of the GFPEPS $G_{\text{GFPEPS}}(\mathbf{k})$ with a given χ . The results are shown in Fig. [3\(a\):](#page-3-0) We find that the error δ in the CM decreases exponentially with the number of bond modes χ . Since all physical quantities depend solely on the CM, our results indicate that if χ is increased, all relevant observables can be approximated by a GFPEPS with exponentially decreasing error. Most importantly, the Hall conductivity $-\overline{(\sigma_{xy}/2\pi)}$ reaches $\overline{C} = -1$ with exponentially decreas-
ing difference, and the entropy of the optimal GEDEDS ing difference, and the entropy of the optimal GFPEPS approximation decreases exponentially with χ .

We have also investigated the power of the GFPEPS to describe topological insulators at finite temperature. This was done by minimizing the free-energy functional $F(\rho_{\text{GFPEPS}}) = \text{tr}(H\rho_{\text{GFPEPS}}) - TS(\rho_{\text{GFPEPS}})$ (S: von Neumann entropy) of the above model at $e_S = 1$, with a GFPEPS with $\chi = 2$, i.e., one bond Majorana fermion per physical fermion. Compare this in Figs. $3(b)$ and $3(c)$. For $T \rightarrow 0$, the entropy of the GFPEPS does indeed converge to zero; that is, it approaches a pure state; its analytical form is just the one given in Eq. [\(5](#page-1-5)), with $\lambda \approx 0.705$. This shows that by minimizing the free energy as a function of shows that by minimizing the free energy as a function of T one can converge to pure states that are topological even for small χ values. Thus, pure GFPEPS are well suited to describe topological insulators in numerical simulations. We have substantiated this claim further by minimizing the free energy $F(\rho_{\text{GFPEPS}})$ for $\chi = 2$ as a function of $-1 \le e_s \le 1$ for $T = 0$; see Fig. [3\(d\).](#page-3-0) The entropies of the optimal GFPEPS were of the order of $\leq 10^{-10}$, which is why their Chern numbers coincide with their Hall conductivities, which jump from 0 to -1 at $e_s \approx 0$. These results indicate that quantum phase
transitions can be detected by approximating the transitions can be detected by approximating the ground-state energy with GFPEPS.

Conclusions.—In this Letter, we have studied whether projected entangled-pair states can be used to describe chiral topological states. We have answered this question in the affirmative by providing a class of GFPEPS describing systems with a nonzero Chern number; these states can be ground states of either gapless strictly local Hamiltonians or gapped Hamiltonians with algebraically decaying hoppings and/or pairings. We have further shown that the gaplessness of the strictly local parent Hamiltonian is a necessary condition to have topological order. Finally, we have numerically studied the ability of GFPEPS to approximate chiral free-fermion systems and found that GFPEPS can efficiently approximate both ground and thermal states of chiral Hamiltonians with a small bond dimension, making them a well-suited tool for the numerical study of chiral fermionic systems.

Whereas we restricted our studies to Gaussian PEPS, it appears that one can also describe interacting chiral systems with fermionic PEPS by twisting the Gaussian PEPS projector $\mathcal E$ with a non-Gaussian map. We therefore believe that fermionic PEPS will also be suitable as a numerical tool to study fractional quantum Hall systems.

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Note added.—After completion of this work, we learned that Dubail and Read had independently obtained related results [[28](#page-4-22)].

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