

Tensor Network Method for Real-Space Topology in Quasicrystal Chern Mosaics

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Computing topological invariants in two-dimensional quasicrystals and supermoiré matter is a remarkable open challenge due to the absence of translational symmetry and the colossal number of sites inherent to these systems. Here, we establish a method to compute local topological invariants of exceptionally large systems using tensor networks, enabling the computation of invariants for Hamiltonians with hundreds of millions of sites, several orders of magnitude above the capabilities of conventional methodologies. Our approach leverages a tensor network representation of the density matrix using a Chebyshev tensor network algorithm, enabling large-scale calculations of topological markers in quasicrystalline and moiré systems. We demonstrate our methodology with two-dimensional quasicrystals featuring C_8 and C_{10} rotational symmetries and mosaics of Chern phases. Our Letter establishes a powerful method to compute topological phases in exceptionally large-scale topological systems, providing the required tool to rationalize generic super-moiré and quasicrystalline topological matter.

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Introduction—Topological phases, although typically characterized by global invariants like the Chern number, can emerge locally in systems lacking translational symmetry [1–10], as well as due to cross-dimensional phenomena in quasicrystals [11,12]. Chern markers allow for characterizing so-called Chern mosaics: spatially alternating local Chern numbers in moiré systems. These topological mosaics have recently been observed in twisted graphene multilayers, where local probes revealed micron-scale domains with alternating Chern numbers of $+1$ and -1 [13]. Topological features are also expected to arise in moiré quasicrystals like 30° twisted bilayer graphene [14–17], twisted graphene trilayers [18,19], twisted transition metal dichalcogenide bilayers [20–22], and generic platforms exhibiting quasicrystallinity or criticality [23–28]. Interfaces between regions with different local Chern markers are expected to host chiral edge modes, forming Chern networks that connect local topological characterization with emergent macroscopic functionalities [29]. However, computing local invariants in exceptionally large systems is a remarkable challenge, as it requires full knowledge of the many-body density matrix, a highly dense object.

Quantum many-body Hamiltonians represent a paradigmatic problem featuring an exponentially large space, whose exact solution becomes quickly unfeasible. Tensor network representations of ground-state wave functions

have enabled obtaining exceptionally accurate solutions to paradigmatic many-body problems [30–52], providing a methodology to accurately solve many-body problems with

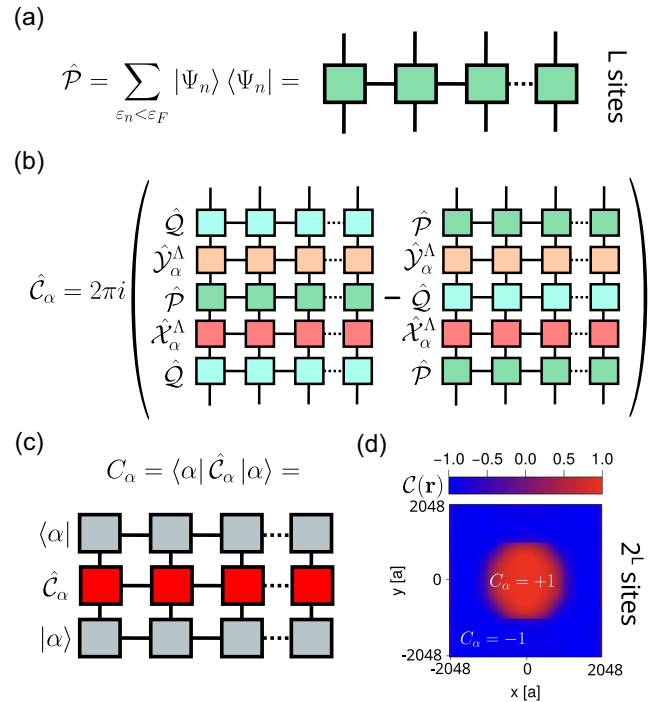


FIG. 1. (a) Tensor network representation of the ground-state projector, computed with a kernel polynomial method. (b) Tensor network construction of the local topological marker. (c) Extraction of the local Chern marker by tensor network contraction. (d) Demonstration for the topological marker for a modulated Chern system with different domains for a system with 16×10^6 sites with a C_∞ symmetric sinusoidal modulation.

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an exponentially large Hilbert space. Recently, tensor network techniques have been extended beyond the realm of quantum many-body physics, finding applications in machine learning [37,53,54], complex dynamics [55–60], ultraprecise function integration [61–64], and exceptionally large electronic problems [65–67]. The ability of tensor networks to represent functions on ultrafine grids [68], makes them a promising technique to compute observables that require storing dense objects in exceptionally large systems.

Here, we establish a tensor network methodology enabling the computation of local topological markers in electronic models of unprecedented size and demonstrate the method for quasicrystalline Chern insulators. This strategy relies on the strategy introduced in Ref. [66], which maps a real-space tight-binding electronic model to a many-body pseudospin model that is solved with a tensor network kernel polynomial method (KPM). This formalism allows for the computation of topological markers in systems with a Hamiltonian too large to be explicitly stored, reaching system sizes on the scale of microns. We demonstrate our methodology depicted in Fig. 1 by applying it to real-space C_8 and C_{10} symmetric modulated π -flux quasicrystal lattices. These modulations result in Chern mosaics emerging across the entire real-space lattice. Our Letter overcomes the finite-size barrier of previous studies for the calculation of local topological invariants, as we perform calculations in systems with up to 268×10^6 sites. We thus introduce a broadly applicable tool for exploring local topological order in quasicrystals and other moiré-patterned quantum materials.

*Tensor network representation of the Chern marker—*Our objective is to compute a real-space topological marker for a large tight-binding Hamiltonian of the form $H = \sum_{\alpha\beta} t_{\alpha\beta} c_{\alpha}^{\dagger} c_{\beta}$, where $c_i^{\dagger}, c_i$ are the creation and annihilation operators in site i . In general, we will focus on Hamiltonians H that do not have translational symmetry, such as those arising from a quasicrystalline modulation of the hoppings due to incommensurate supermoiré patterns. For systems with hundreds of millions of sites, H becomes too large to even be stored. Using our methodology, we reinterpret a 2^L -site Hamiltonian as a many-body operator of an auxiliary many-body pseudospin chain of L sites, for which the index s, s' corresponds to an element of a pseudospin many-body basis as $s \equiv (s_1, s_2, \dots, s_L)$ and $s' \equiv (s'_1, s'_2, \dots, s'_L)$. In this form, the Hamiltonian can be written using a tensor network representation as a matrix product operator (MPO) in the pseudospin basis as introduced in Ref. [66],

$$\hat{H} \equiv \sum \Gamma_{s_1, s'_1}^{(1)} \Gamma_{s_2, s'_2}^{(2)} \Gamma_{s_3, s'_3}^{(3)} \cdots \Gamma_{s_L, s'_L}^{(L)} c_s^{\dagger} c_{s'}, \quad (1)$$

where $\Gamma_{s_i, s'_i}^{(n)}$ are tensors of dimension χ_n , the bond dimensions of the MPO [69].

Topological invariants, typically defined in momentum space through quantities like the Chern number [70,71], fail in nonperiodic systems such as quasicrystals or disordered lattices, where real-space markers instead capture spatially resolved topological order [1,2,72,73], remaining applicable to disordered, interacting, and higher-dimensional systems [7], as well as real-space formulations of quantum geometry [74–78].

The usual Chern marker is defined at any position α at the cost of the local spectral projectors into occupied states $\hat{P}$ and unoccupied states $\hat{Q} = \hat{1} - \hat{P}$ as

$$C_{\alpha} = 2\pi i \langle \alpha | \hat{Q} \hat{X} \hat{P} \hat{Y} \hat{Q} - \hat{P} \hat{X} \hat{Q} \hat{Y} \hat{P} | \alpha \rangle, \quad (2)$$

where $\hat{X}$ and $\hat{Y}$ are the position operators. In translationally invariant systems, C_{α} converges to the global Chern number in the bulk, while for inhomogeneous systems, C_{α} reveals the spatial structure of topological order, including the presence of different topological domains, leading to the possibility of diagnosing the presence of a Chern mosaic.

In the following, we cast this local Chern marker into a tensor network representation by evaluating the ground-state projector $\hat{P}$ via a Chebyshev expansion using tensor networks [27,51,52]. At zero temperature, the ground-state projector is in exact correspondence with the density matrix, which can be written as an MPO,

$$\hat{P} = \int_{-\infty}^{\epsilon_F} \delta(\omega - \hat{H}) d\omega = \sum \Xi_{s_1, s'_1}^{(1)} \Xi_{s_2, s'_2}^{(2)} \cdots \Xi_{s_L, s'_L}^{(L)} |s\rangle \langle s'|, \quad (3)$$

where $\Xi_{s_i, s'_i}^{(n)}$ are the tensors representing $\hat{P}$, as graphically represented in Fig. 1(a). The explicit construction of the ground-state projector with usual matrices is highly demanding. For sparse Hamiltonians, Chebyshev methods allow for calculation of the LDOS at specific sites, since it can be computed using Chebyshev moments μ_n^{α} locally at a site α using matrix-vector contractions. However, storing the full projector $\hat{P}$ is impossible even for modestly sized systems since the operator $\hat{P}$ is dense and therefore takes up memory that scales quadratically in the total number of atoms of the system. For example, for a lattice of $10^3 \times 10^3$ atoms, one would generically need to store 1×10^9 complex numbers and do algebra operations with a dense matrix of size $10^6 \times 10^6$. Using our method, however, the MPO representation is achievable both for sparse and dense matrices, and hence, one can make use of it to create a compressed and computationally manageable version of the density matrix $\hat{P}$, which can be stored as a tensor network taking up only logarithmically increasing memory as a function of system size. This technique for compression has been leveraged for a variety of single-particle Hamiltonians [57,58,60,66,67,79], as well as in the context

of Green's functions [80,81]. Here, we focus on π -flux quasicrystalline square lattice systems with up to 268×10^6 sites.

We now elaborate on the construction of the Hamiltonian as a tensor network. A generic single-particle tight-binding Hamiltonian can be written in tensor network form as $\hat{\mathcal{H}} = \sum_n \hat{\mathcal{B}}_n \mathbb{A}(n) + \text{H.c.}$, where $\mathbb{A}(n)$ corresponds to an MPO representation of the matrix with elements $\delta_{i,i+n}$, and $\hat{\mathcal{B}}_n$ corresponds to a diagonal MPO representing a matrix with elements $\langle i | \hat{\mathcal{B}}_n | i \rangle = \hat{H}_{i,i+n}$. For instance, in the simple case where the Hamiltonian corresponds to a one-dimensional tight-binding chain, $\hat{\mathcal{B}}_n$ would yield the n th nearest neighbor hoppings. In two or higher dimensional models, it becomes necessary to reshape the lattice into a periodically broken 1D chain with long range hoppings. The structure of the off-diagonals of the Hamiltonian matrix must therefore be reflected in the MPO $\hat{\mathcal{B}}_n$. In general, these MPOs can be constructed in one of two ways: (i) constant or periodically broken MPOs can be constructed exactly as outlined below; (ii) modulated or otherwise spatially varying structures can be constructed by mapping the real-space structure of the desired Hamiltonian off-diagonal and constructing a function $B_n(i) = H_{i,i+n}$, from which the MPO can be recovered using the quantum tensor cross interpolation (QTCI) algorithm [61–64]. In essence, this approach combines a binary encoding of lattice coordinates with low-rank tensor interpolation, yielding an exponentially large effective grid at only polynomial cost. Furthermore, the $\mathbb{A}(n)$ operators can be constructed for any n : the one-site translation operator can be defined explicitly using $\mathbb{A}(1) = \sum_l^L (\sigma_l^+ \otimes_{m>l} \sigma_m^-)$. From this expression, all $\mathbb{A}(n)$ operators can be calculated in polynomial time by decomposing $n = \sum_i 2^{l_i}$, and computing $\mathbb{A}(2^{l_i})$ recursively as $\mathbb{A}(2^{l_i}) = \mathbb{A}(2^{l_i-1}) \cdot \mathbb{A}(2^{l_i-1})$, which in the worst case scenario has to be done $L - 1$ times. After this recursive calculation, one can simply take the product $\mathbb{A}(n) = \prod_i \mathbb{A}(2^{l_i})$. In the case of a two-dimensional model, for instance, one can think of a $2^{L_x} \times 2^{L_y}$ Hamiltonian as a chain, periodically interrupted every 2^{L_x} sites, with long range neighbors connecting over a distance of 2^{L_x} atoms. The Hamiltonian would contain two terms $\mathbb{A}(1)\mathbb{S} + \mathbb{A}(2^{L_x})$. The inclusion of the MPO $\mathbb{S} = 1 - \otimes_l^L \mathbb{1}_l \prod_{m>L_y} (\mathbb{1}_m - \sigma_m^z)/2$ produces the correctly interrupted hopping structure. Generically, this tensor network representation allows us to perform the KPM expansion directly at the level of Chebyshev polynomials of the Hamiltonian MPO $\hat{\mathcal{H}}$ [27,50–52,65,66], yielding the density matrix in MPO form as

$$\begin{aligned} \hat{\mathcal{P}} &= \sum_{n=0}^{N_c} T_n(\hat{\mathcal{H}}) \int_{\varepsilon_F}^1 d\omega \frac{T_n(\omega)}{\sqrt{1-\omega^2}} \\ &= \arccos(\varepsilon_F) \mathbb{1} + \sum_{n=1}^{N_c} \frac{\sin[n \arccos(\varepsilon_F)]}{n} T_n(\mathcal{H}), \end{aligned} \quad (4)$$

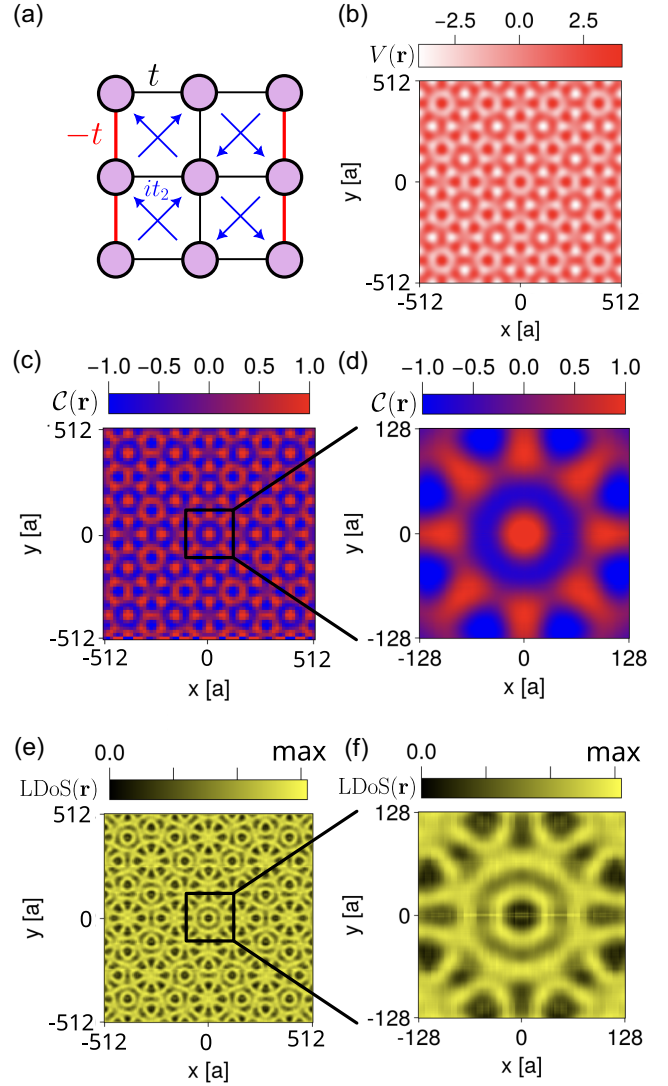


FIG. 2. (a) Schematic representation of the π -flux model with nearest neighbor hopping t and second nearest neighbor imaginary hopping it_2 (b) C_8 symmetric modulation of the second nearest neighbor hopping $t_2 = t_2^{(0)} V(r)$. (c) Quasicrystal Chern mosaic obtained from the MPO-KPM method across a $2^{10} \times 2^{10}$ (1×10^6) atom lattice. (d) Enlargement of the central 256×256 atoms. (e) Local density of states of the Chern network resulting from the topological domains across the entire system. (f) Enlargement of the central 256×256 atoms.

where $T_n(x)$ are the Chebyshev polynomials with recursion relation $T_n(x) = 2xT_{n-1}(x) - T_{n-2}(x)$ with $T_0 = 1$ and $T_1(x) = x$ [82], and N_c is the total number of Chebyshev polynomials used in the expansion. The upper limit of the integral is set to 1 since the Hamiltonian is rescaled so that its spectrum has support in the interval $\omega \in [-1, 1]$ where the orthonormality relations of the Chebyshev polynomials hold.

We now elaborate on the tensor network representation of position operators. We can make use of the QTCI algorithm [83,84] to construct diagonal MPOs for the position operators $\hat{X}$ and $\hat{Y}$, yielding $\hat{\mathcal{X}}$ and $\hat{\mathcal{Y}}$, respectively.

These could then be used to construct a topological marker MPO $\hat{C} = 2\pi i(\hat{Q}\hat{X}\hat{P}\hat{Y}\hat{Q} - \hat{P}\hat{X}\hat{Q}\hat{Y}\hat{P})$ in analogy with Eq. (2). However, while this expression can accurately be used with dense matrices and is mathematically exact, it is not optimal for tensor network calculations. Firstly, even though MPOs $\hat{X}$ and $\hat{Y}$ generically exhibit low bond dimensions when constructed from the QTCI algorithm, their products with the density matrix generate objects with a very large bond dimension, leading to difficulties with computational speed of calculations. On the other hand, for a tight-binding model with 2^L sites, the diagonal elements of $\hat{X}$ will themselves grow to $\mathcal{O}(2^{L-1})$. This will lead to an amplification of errors stemming from the tensor network representing $\hat{P}$, by a factor that will increase when moving away from the center of the lattice, possibly accounting for the growth in bond dimension when computing $\hat{P}$ or $\hat{Q}$. These issues can be resolved for tensor network based calculations by recasting the calculation of the global topological marker MPO with quenched position operators. In particular, one can first center the position operators relative to the site α where one wishes to compute the marker's value. In addition one can bound the position operator by approximating $\hat{X} \approx \Lambda \sin(\hat{X}/\Lambda)$ for $x/\Lambda \ll 1$. The value of Λ needs to be sufficiently large when compared to the correlation length of the topological operator such that the small angle approximation holds for a region that is wide enough to capture the local environment of the site i correctly when taking products involving $\hat{P}$ and $\hat{Q}$ [85]. This suppresses the increase in bond dimension while retaining enough information to accurately predict the Chern marker. Replacing $\hat{X} \rightarrow \tilde{X}_\alpha^\Lambda = \Lambda \sin((\hat{X} - x_\alpha)/\Lambda)$ and equivalently $\hat{Y} \rightarrow \tilde{Y}_\alpha^\Lambda$, we can approximately compute the local Chern marker as

$$C_\alpha = 2\pi i \langle \alpha | \hat{Q} \tilde{X}_\alpha^\Lambda \hat{P} \tilde{Y}_\alpha^\Lambda \hat{Q} - \hat{P} \tilde{X}_\alpha^\Lambda \hat{Q} \tilde{Y}_\alpha^\Lambda \hat{P} | \alpha \rangle, \quad (5)$$

or as graphically depicted in Figs. 1(b), 1(c) and therefore resolve C_α across systems with hundreds of millions of sites. An example for a simple circular sinusoidal modulation is given in Fig. 1(d). A benchmarking of the convergence of the Chern marker for the Haldane model is given in Supplemental Material [86], where this method is compared against a standard approach based on dense matrices.

Quasicrystalline Chern mosaic—We now use the previous methodology to resolve the topological domains of an exceptionally large two-dimensional quasicrystal. The π -flux model on the square lattice provides a paradigmatic realization of Dirac fermions in a two-dimensional system [87]. In this model, each plaquette of the square lattice is threaded by a magnetic flux of π , leading to a nontrivial hopping phase structure, whose Hamiltonian reads $H_1 = -t \sum_{\langle \alpha, \beta \rangle} e^{iA_{\alpha\beta}} c_\alpha^\dagger c_\beta + \text{H.c.}$ A convenient choice of

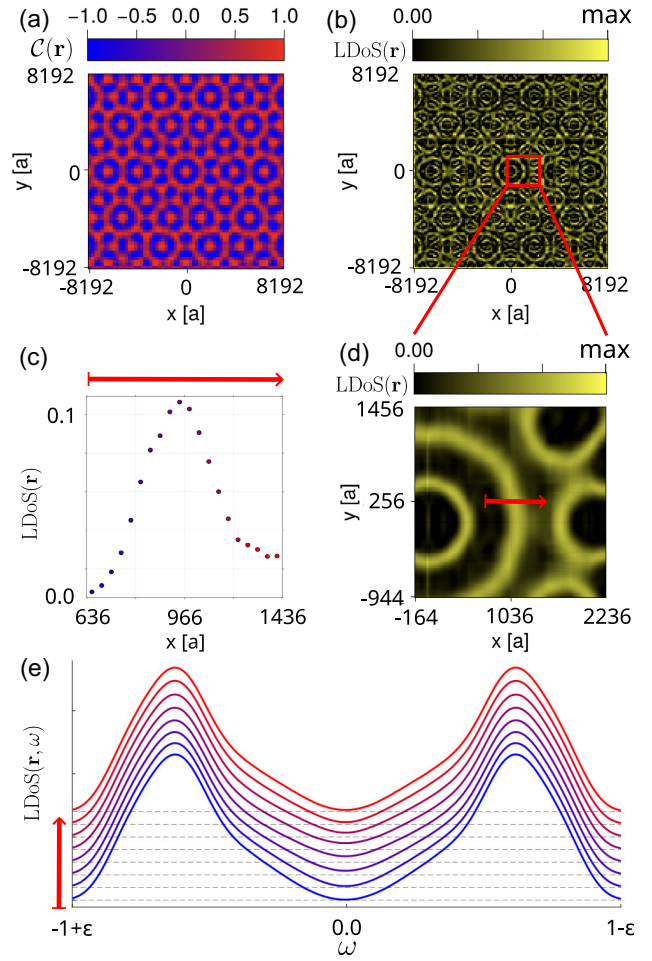


FIG. 3. (a) Local Chern marker obtained from the MPO-KPM method across a C_{10} symmetric modulated lattice of $2^{14} \times 2^{14}$ (268×10^6) atoms. (b) In-gap LDOS showcasing the presence of Chern network with a C_{10} symmetric pattern. (c) LDOS along a path crossing an edge state. (d) Enlargement of a 2400×2400 atom region containing the path of panel (c). (e) LDOS as a function of frequency for points along the same path calculated using KPM [66].

gauge $A_{\alpha\beta}$ assigns alternating signs to the hoppings along one direction as shown in Fig. 2(a). For a periodic system, this yields a Dirac model with two cones, for which topological phases can be induced by adding next-nearest-neighbor imaginary hoppings that break time-reversal symmetry as $H_2 = it_2 \sum_{\langle\langle \alpha, \beta \rangle\rangle} \nu_{\alpha\beta} c_\alpha^\dagger c_\beta$, where $\nu_{\alpha\beta} = \pm 1$ depends on the hopping direction. This term opens a gap at the Dirac points and turns the system into a Chern insulator with Chern number $C = \text{sign}(t_2)$. We now apply our method to compute the local Chern marker to modulated π -flux models. We take $t_2 = t_2^{(0)} V(\mathbf{r})$ with $V(\mathbf{r}) = V_0 \sum_{i=1}^n \cos(\mathbf{q}_i \cdot \mathbf{r})$, with $t_2^{(0)} = 0.2t$ and $V_0 = 1/2$, and set $n = 4$ or 5 , corresponding to C_8 and C_{10} symmetries. We use a modulation period of about 80 atomic sites for Fig. 2, such that $|\mathbf{q}_i| = 2\pi/80$, yielding

topological domains with characteristic width on the order of 40 atoms. For Fig. 3 we use a modulation period of 1080 atoms. In both Figs. 2(c), 2(d) for the C_8 modulation and Fig. 3(a) for the C_{10} case, we observe a quantization of the local marker to a very good degree. In general, the results reveal the presence of quasicrystalline Chern mosaics emerging due to the incommensurate geometry.

Quasicrystalline Chern network—We now address the topologically protected edge states occurring at every boundary between topological domains in the quasicrystal Chern mosaic. At half-filling within the current model, the intricate nature of the C_8 and C_{10} symmetric quasicrystalline Chern networks become evident in the local density of states, shown in Figs. 2(e), 2(f), and 3(b)–3(d). This Chern network results in an enhancement of the in-gap density of states due to the presence of chiral in-gap edge states propagating along the bulk of the sample, as seen in Figs. 3(c) and 3(e). Furthermore, it is worth noting that this Chern network percolates through the entire sample in Figs. 2(e), 2(f) and 3(b), 3(d), which would enable topologically protected conduction channels at a macroscopic scale.

Conclusion—Computing topological invariants of non-periodic quantum systems, including quasicrystal and supermoiré materials is an exceptional challenge due to the large sizes of these systems. Here, we have demonstrated a tensor network methodology that enables computing local Chern numbers in real space for exceptionally large models. Our methodology relies on creating a tensor network representation of the topological marker with a tensor network Chebyshev expansion of the Hamiltonian. This methodology enables computing topological invariants of exceptionally large models, and in particular models whose single-particle Hamiltonian is too large to be stored explicitly. We exemplified our methodology with C_8 and C_{10} symmetric quasicrystals, demonstrating that our methodology enables faithfully computing topological domains, whose impact can be directly observed in the resulting network of topological in-gap modes. Our approach can be extended to compute topological invariants in supermoiré systems, including valley Chern numbers, $\mathbb{Z}_2$ quantum spin Hall indices, crystalline Chern numbers, and real-space quantum geometry, providing a general framework for analyzing topological states in large-scale supermoiré matter.

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Data availability—The data that support the findings of this article are openly available [88].

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