Band Theory and Boundary Modes of High-Dimensional Representations of Infinite Hyperbolic Lattices

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(Received 28 March 2022; revised 22 June 2022; accepted 27 July 2022; published 18 August 2022)

Periodic lattices in hyperbolic space are characterized by symmetries beyond Euclidean crystallographic groups, offering a new platform for classical and quantum waves, demonstrating great potential for a new class of topological metamaterials. One important feature of hyperbolic lattices is that their translation group is nonabelian, permitting high-dimensional irreducible representations (irreps), in contrast to abelian translation groups in Euclidean lattices. Here we introduce a general framework to construct wave eigenstates of high-dimensional irreps of infinite hyperbolic lattices, thereby generalizing Bloch's theorem, and discuss its implications on unusual mode counting and degeneracy, as well as bulk-edge correspondence in hyperbolic lattices. We apply this method to a mechanical hyperbolic lattice, and characterize its band structure and zero modes of high-dimensional irreps.

DOI: 10.1103/PhysRevLett.129.088002

Introduction.—Bloch's theorem has been the foundation of solid-state physics. From the concept of energy bands to the blossoming field of topological insulators, everything starts with how wave eigenstates are modulated by spatially periodic potentials in crystals. The abelian nature of the translation groups in crystals limits their representations to one-dimensional (1D), i.e., the Bloch factor, e^{ikr}, greatly simplifying the mathematical description of waves in crystals.

New materials and structures with complex spatial order beyond periodic lattices are being discovered, with a particularly interesting class being hyperbolic lattices, which have recently evolved from pure mathematical concepts [1] to real materials realizable in the lab [2–12]. These lattices are perfectly ordered in hyperbolic space, i.e., space with constant negative curvature. A simple example of a 2D hyperbolic lattice is the tiling of regular heptagons where three heptagons meet at each vertex (i.e., the {7,3} tiling). The interior angle of a heptagon in a flat plane is greater than $2\pi/3$, leading to an obvious frustration. This frustration is resolved on a hyperbolic plane, where the interior angle is modified by the Gaussian curvature. Interestingly, in contrast to limited choices of regular lattices in Euclidean space, there are infinitely many regular lattices in hyperbolic space, opening up a huge space for unconventional symmetries and physics.

How to describe waves in hyperbolic lattices? In recent studies, a range of intriguing features has been reported, e.g., topological edge states [5,11], higher-genus torus Brillouin zones (BZs) [6,9], and circuit quantum electrodynamics [2–4,12], outlining an exciting arena of new theories. However, key questions still remain about the fundamental principles of constructing wave eigenstates from the symmetries of these hyperbolic lattices. As mentioned above, the simple form of the Bloch factor comes from the abelian translation group in Euclidean space. In hyperbolic lattices, in contrast, translations form an infinite nonabelian group, calling for high-dimensional irreducible representations (irreps). How to construct waves of these high-dimensional irreps, and the fundamental physics of the resulting waves, remain open questions. An alternative way to demonstrate the necessity of high-dimensional irreps in hyperbolic lattices is the scaling of the number of wave modes with the system size. A Euclidean lattice of linear size L with n degrees of freedom (d.o.f.s) per unit cell has n bands in reciprocal (k) space, and the number of points in the first BZ is L^D (where D is the spatial dimension), making the number of d.o.f.s in real space and k space equal. In a hyperbolic lattice, however, the number of unit cells grows *exponentially* with L, leading to $\mathcal{O}(e^L)$ wave modes, which is much greater than the number of points in the first BZ. As we analyze in this Letter, this indicates that a sequence of high-dimensional irreps is needed to define a complete basis of waves on hyperbolic lattices at large L.

In this Letter, we introduce a generalized Bloch's theorem for high-dimensional irreps of the nonabelian translation groups of infinite hyperbolic lattices, which allows us to construct wave eigenstates for any given high-dimensional irreps on hyperbolic lattices, and we discuss the unusual physics of these waves. We find that $d \times n$ bands of bulk waves arise from d-dimensional unitary irreps in hyperbolic lattices (in contrast to n bands in Euclidean lattices). In addition, spatially localized edge or interface modes must involve high-dimensional irreps. We apply this formulation to a hyperbolic mechanical lattice, and reveal a series of unusual features from zero modes in hyperbolic lattices where the bulk is overconstrained, to a modified bulk-edge correspondence for potential topological states in hyperbolic space.

Wave basis of high-dimensional representations of hyperbolic lattices.—In this section we consider general principles for constructing wave basis from lattice potentials. Let us first briefly review the case of Euclidean lattices, where wave eigenstates are described by Bloch's theorem. Because the translation group T of Euclidean lattices is abelian and all elements of T commute with the Hamiltonian H (which has the same periodicity of the lattice), one can choose a set of waves that are eigenstates of H and all elements t_R in T

$$t_R\psi(r) \equiv \psi(t_R^{-1}r) = \psi(r)e^{ikR}, \tag{1}$$

and these waves can be written as

$$\psi(r) = e^{-ikr}u(r), \tag{2}$$

where r is the position in space, k is the crystal momentum, and $u(r)$ is a function with the same periodicity as that of the lattice. This theorem from Bloch [Eq. (2)] has an equivalent description, using the Wannier basis, a complete orthogonal basis that characterizes localized molecular orbitals of crystalline systems [13],

$$\psi(r) = \sum_R \phi_R(r)e^{-ikR} = \sum_{t_R\in T}[t_R\phi(r)]e^{-ikR}, \tag{3}$$

where the Wannier function $\phi_R(r)$ obeys $\phi_R(r) = t_R\phi(r) = \phi(t_R^{-1}r)$. The sum here is over all lattice vectors (or equivalently all elements of the lattice translation group). These three formulas [Eqs. (1)–(3)] are equivalent to each other.

Next, we generalize this formulation to hyperbolic lattices in the form of $\{p,q\}$ tilings (i.e., lattices of p-sided polygons tiling the hyperbolic plane in a regular pattern such that q polygons meet at each vertex). The space symmetries of these tilings are described by the Coxeter group G, a nonabelian infinite group which is analogous to the space group of Euclidean lattices [14]; see the Supplemental Material for a brief summary. For tilings that satisfy the condition that q has a prime divisor less than or equal to p, a *generalized translation subgroup* $T\subset G$ can be defined, where each element $t\in T$ has a one-to-one correspondence with each polygon in the tiling [15], and the lattice dual to the tiling (i.e., $\{q,p\}$) can be defined as a *generalized Bravais lattice*. This algebraic generalization of translations and Bravais lattices recovers the conventional definition when applied to regular Euclidean Bravais lattices. Similar to the Euclidean case, lattices that do not satisfy this criterion (non-Bravais lattices) can be considered as a Bravais lattice with a basis (internal d.o.f.s). This definition differs slightly from the one used in Ref. [10], because our translation group is not limited to hyperbolic translations, and it broadens Bloch's theorem to more generic non-Euclidean lattices (e.g., spherical lattices like the 600 cells [16]).

This generalized translation group enables a generalization of Bloch's theorem to higher-dimensional irreps. To achieve this, we start by drawing analogies with Eqs. (1) and (3). Here, although the Hamiltonian H commutes with all elements of T, the group T itself is nonabelian. Thus, some eigenstates of H must lie in some high-dimensional irreps of T. That is, if $\psi_1(x)$ is an eigenstate of H with energy E, there must be an irrep ρ (say d dimensional) and $d-1$ other eigenstates $\psi_2(x),\ldots,\psi_d(x)$ with the same energy E such that $\forall\ t\in T$

$$t\psi_j(r) \equiv \psi_j(t^{-1}r) = \psi_i(r)\rho(t)_{ij}, \tag{4}$$

where the $d\times d$ matrix $\rho(t)$ is a d-dimensional irrep of the translation group T [17]. This is the nonabelian generalization of Eq. (1), and the d degenerate eigenstates $\psi_i(r)$ are the *generalized Bloch waves*. This definition has been adopted in Ref. [9] to characterize eigenstates on finite hyperbolic lattices under periodic boundary conditions. Here we show how such waves can be constructed for general infinite hyperbolic lattices, leading to band structures. In particular, we use the Wannier basis in analogy to Eq. (3),

$$\psi_j(r) = \sum_{t\in T}[t\phi_i(r)]\rho(t^{-1})_{ij}, \tag{5}$$

where a set of d Wannier functions $\phi_i(r)$ can be obtained by solving the eigenstates of the Hamiltonian (see the next section). It is straightforward to verify that waves constructed via Eq. (5) indeed transform as Eq. (4) (see Supplemental Material).

Below, we show that for each irrep, all of its eigenmodes can be obtained using this generalized Bloch's theorem. By exploring all irreps of T, a complete description of all eigenmodes can in principle be obtained.

Eigenmodes in non-Euclidean lattices.—In this section we apply the generalized Bloch theorem to find eigenmodes of any high-dimensional irrep $\rho(t)$. In general, we can write any states as

$$|\psi\rangle = \sum_{t\in T}\sum_{a=1}^{n} c(t,a)|v_t^{(a)}\rangle. \tag{6}$$

Here we label each unit cell using elements of the translation group $t\in T$, and $|v_t^{(a)}\rangle$ is a complete orthonormal basis for the n d.o.f.s (labeled by a) in unit cell t. In the continuum, the index a is a continuous variable labeling coordinate r (plus some additional indices for internal d.o.f.s). One convenient choice of basis is to require $|v_t^{(a)}\rangle = t|v_I^{(a)}\rangle$, where the basis in the unit cell I at the origin can be chosen arbitrarily as $|v_I^{(a)}\rangle = |v^{(a)}\rangle$ and then the basis of any other unit cell is obtained via a translation. Due to the one-to-one correspondence between group elements of T and unit cells, this approach defines a unique set of basis $|v_t^{(a)}\rangle$. In this basis, $|v_t^{(a)}\rangle$ can effectively be decomposed into the direct product of $|v_t^{(a)}\rangle = |v^{(a)}\rangle \otimes |t\rangle$, where $|t\rangle$ labels the unit cell and $|v^{(a)}\rangle$ spans the linear space of d.o.f.s in a unit cell. As a result, any Hamiltonian (or dynamical matrix) that preserves the lattice translational symmetry can be written in the following form:

$$H = \sum_{t' \in T} \mathcal{H}_{t'} \otimes \sum_{t \in T} |t\rangle\langle tt'|, \tag{7}$$

where $\mathcal{H}_{t'}$ is an $n \times n$ matrix defined in the linear space of $|v^{(a)}\rangle$. It describes the hybridization between unit cells t and tt'. If H is Hermitian, $\mathcal{H}_{t'} = \mathcal{H}^{\dagger}_{(t')^{-1}}$.

Following the generalized Bloch's theorem discussed above [Eq. (5)], we write the Bloch-wave eigenstates of a d-dimensional irrep,

$$|\psi_j\rangle = \sum_{t \in T} \left[\sum_{a=1}^{n} \lambda_{a,i} |v^{(a)}\rangle \otimes |t\rangle \right] \rho(t^{-1})_{ij}. \tag{8}$$

Using this construction, the eigenvalue problem $H|\psi_j\rangle = E|\psi_j\rangle$ is converted to the eigenvalue problem of a $dn \times dn$ matrix $H(\rho)\lambda = E(\rho)\lambda$ where

$$H(\rho) = \sum_{t \in T} \mathcal{H}_t \otimes \rho(t^{-1})^T. \tag{9}$$

Each eigenvalue give us an eigenenergy E, and the corresponding eigenvector $\lambda_{a,i}$ yields d degenerate Bloch waves, carrying this d-dimensional irrep [Eq. (8)]. It is important to highlight that for each d-dimensional irrep, we shall obtain $d \times n$ eigenenergies, i.e., $d \times n$ energy bands, each d-fold degenerate ($d^2 \times n$ eigenstates in total). This is in sharp contrast to Euclidean lattices, where the band number is determined solely by n, because $d = 1$. The fact that $d^2 \times n$ eigenstates emerge here, instead of n, is analogous to the regular representation of a finite group [17], where a d-dimensional irrep reoccurs d times and thus $\sum_{\text{irreps}} d^2 =$ the number of group elements. A similar procedure can be done solving eigenstates in the continuum, as described in the Supplemental Material.

Phonons on {14,7}.—We now demonstrate the principles discussed above in a particular hyperbolic lattice: the {14,7} tiling (Fig. 1). The translation group T of {14,7} can be generated by the hyperbolic translations that translate the central 14-gon to its neighbors, $\{\gamma_i\}_{i=1}^{7}$, as shown in Fig. 1 on the Poincaré disk model (which maps the infinite hyperbolic plane to the unit disk $\mathbb{D}$) [18]. It is straightforward to see that

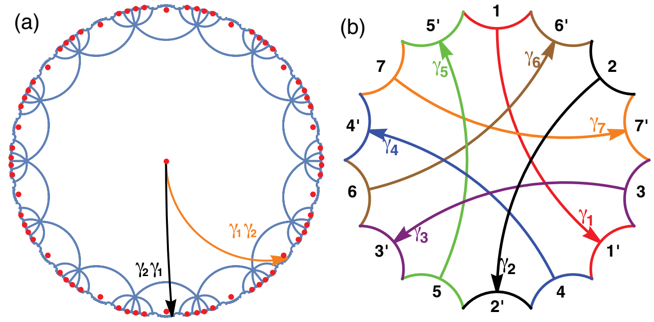

FIG. 1. The Bravais lattice and translation group of a 2D hyperbolic periodic tiling {14,7}. (a) The {14,7} tiling (blue geodesics showing the edges) and its dual lattice {7,14} (red dots showing the nodes) on the Poincaré disk. The {7,14} is a generalized Bravais lattice. The two arrows mark translations $\gamma_2\gamma_1$ and $\gamma_1\gamma_2$ respectively, demonstrating the noncommutativity of translations. (b) Seven translations, $\gamma_1, \ldots, \gamma_7$, denoted as arrows on a 14-gon, which generates the translation group of the {14,7} tiling.

this is a nonabelian group, i.e., operations γ_i do not commute with one another (example shown in Fig. 1). Acting products of γ_i generate all 14-gons without overlapping on the {14,7}, and they must satisfy two constraints, $\gamma_5\gamma_2\gamma_6\gamma_3\gamma_7\gamma_4\gamma_1 = 1$ and $\gamma_5\gamma_3\gamma_1\gamma_6\gamma_4\gamma_2\gamma_7 = 1$. By identifying edges i with i', a 14-gon becomes a genus-3 torus Σ_3 [19], and each γ_i becomes a loop on this torus, i.e., one element of the fundamental group $\pi_1(\Sigma_3) = \{\langle a_1, a_2, a_3, b_1, b_2, b_3\rangle, [a_1, b_1][a_2, b_2][a_3, b_3] = 1\}$ (here $[t, t'] \equiv tt't^{-1}t'^{-1}$ is the commutator between two group elements). Based on this mapping, an isomorphism between T and $\pi_1(\Sigma_3)$ can be obtained (see Supplemental Material [20]), utilizing the relation between the deck group of universal covers and fundamental groups [21]. Thus we can use d-dimensional irreps of the a's and b's to construct irreps of T.

Here, we use an explicit model mechanical system to demonstrate the principles discussed above. More examples using tight-binding models can be found in the Supplemental Material [20]. We place a mass $m = 1$ at each node of {7,14} [red dots of Fig. 1(a)] and use an elastic spring (with spring constant $k = 1$) to connect neighboring nodes. This spring network has two (in plane) degrees of freedom per unit cell ($n = 2$); thus for modes in 1D representations of T, we expect two phonon bands, which is indeed what we observe in Fig. 2(a). Here, 1D representations span a six-dimensional BZ (from the six generators a's and b's), and we plot a 1D cut of this 6D space using the representation $a_1 = e^{ik}$ and $a_2 = a_3 = b_1 = b_2 = b_3 = 1$.

For higher-dimensional irreps, the BZ is generalized to a $[(2g - 2)d^2 + 2]$-dimensional space ($g = 3$ for {14,7}) [9], which labels all d-dimensional irreps. Here, to demonstrate the generalized Bloch's theorem for higher-dimensional irreps, we plot a 1D cut of this 18-dimensional band structure using this set of 2D irreps:

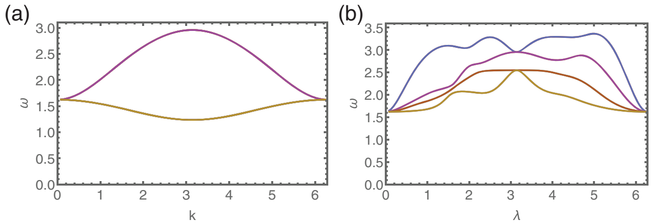

FIG. 2. Phonon band structure of a hyperbolic spring network on {7,14}. (a) A 1D cut of phonon bands from 1D representations, where each wave vector k labels a 1D representation of T. Same as in Euclidean lattices, the number of bands (2) coincides with the number of d.o.f.s per unit cell $n = 2$. (b) A 1D cut of phonon bands from 2D irreps, where each λ marks one 2D irrep [Eq. (10)]. Here, the band number is $d \times n = 4$ instead of $n = 2$, and each band is twofold degenerate.

$$a_\alpha = \cos \lambda I + i \sin \lambda \sigma_\alpha, \qquad b_1 = b_2 = I, \qquad b_3 = e^{-i\lambda} I, \tag{10}$$

where I is the 2×2 identity matrix and σ_α with $\alpha = 1, 2, 3$ are the three Pauli matrices. For $0 < \lambda < \pi$ or $\pi < \lambda < 2\pi$, each λ labels a 2D irrep, and we can compute its eigenfrequencies and eigenmodes following the generalized Bloch theorem [Fig 2(b); see Supplemental Material [20] for details]. Indeed, we found $d \times n = 4$ phonon bands, each twofold degenerate.

Nonunitary representations and bulk-edge correspondence.—In this section, we discuss states with localized edge modes. Although the origin of such edge modes may vary (e.g., topological or accidental), they all involve nonunitary representations of the translation groups. In Euclidean space, a wave from a nonunitary representation takes the same form as the Bloch wave $\psi(r) = u(r)e^{-ikr}$, but its wave vector k takes a complex value. In general, in a Euclidean lattice, any bulk (edge) modes can be written as the superposition of unitary (nonunitary) modes, which correspond to a Fourier (Laplace) transformation.

In hyperbolic Bravais lattices, edge modes also involve nonunitary representations, but interestingly, they cannot be described by 1D nonunitary representations of the translation groups, due to the nonabelian nature of T. For any 1D representation, although repeatedly acting one translation t with $\rho(t)^\dagger \neq \rho(t)^{-1}$ does lead to coherent decay (or growth) of its amplitude [Fig. 3(b)], the mode must be invariant under any translation that belongs to the commutator subgroup of the translation group [Fig. 3(c)]. The commutator subgroup $[T, T]$ is generated by all commutators $[t, t']$ of group elements of T, and for any 1D representations, $\rho([t, t']) = 1$, i.e., these modes must be invariant under $[t, t']$ (as shown in the Supplemental Material [20]). In contrast to Euclidean lattices, where $[T, T]$ is always trivial, the commutator subgroup of a hyperbolic lattice contains infinitely many translations in various directions, along which 1D-representation modes cannot decay, making it impossible to form a localized edge state (although certain corner modes are allowed, e.g., at the tip of a sharp wedge along the orange geodesic in Fig. 3 where the mode grows exponentially toward the tail of the arrow).

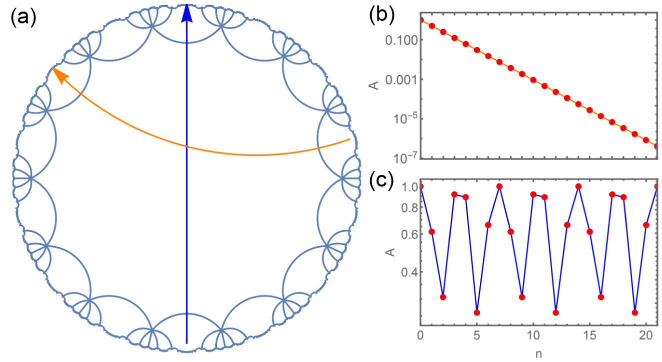

FIG. 3. Absence of localized modes in 1D representations. (a) Two types of geodesics in {14,7} constructed by repeatedly acting on the central 14-gon via either (i) one generator (γ_7^{-1} in this case, orange) or (ii) an element in $[T, T]$ (blue). (b),(c) Amplitude of a zero mode (see Supplemental Material [20]) from a nonunitary 1D presentation on discrete degrees of freedom in unit cells for these two geodesics, where the mode exponentially decays on type (i) geodesics (b), and oscillates on type (ii) geodesics (c). The periodicity in (c) is a universal feature of all 1D representation modes.

This observation has a deep impact on topological edge-bulk correspondence. In Euclidean space, it has long been know that a nontrivial topological structure in bulk band can lead to nontrivial edge modes, known as the bulk-edge correspondence [22]. For a hyperbolic lattice, such correspondence necessarily requires higher-dimensional representations. Even if a bulk topological index only involves 1D representations (e.g., Ref. [11]), the corresponding edge states (if exist) must involve higher-dimensional nonunitary irreps, because 1D (unitary and nonunitary) representations cannot form edge modes. This observation is one example demonstrating the incompleteness of 1D representations in non-Euclidean lattices. In fact, because 1D representations (unitary or not) can only lead to waves invariant under any transition in $[T, T]$, they cannot offer a complete wave basis. Any modes (bulk or edge) not obeying this invariance necessarily require higher-dimensional irreps.

Another interesting feature that arises by considering nonunitary representations is the existence of zero modes. Although the mechanical lattice we consider here has coordination number $z = 14$, which is far above the Maxwell criterion for stability [23–26], the lattice is guaranteed to have zero modes under open boundary conditions. This can be seen, e.g., in 1D representation, by comparing the number of constraints (7 per unit cell from the springs) and free variables (13 from 6 complex momenta $k_1, \ldots, k_6$ and 1 for the direction of displacements; see Supplemental Material [20] for details). The excess free variables allows zero modes in the linear model, in a way similar to how corner modes arise in overconstrained lattices

[27]. This works similarly for 2D irreps where we have 18 complex momenta. An alternative way to see the existence of these zero modes is that the fraction of boundary nodes is $\mathcal{O}(1)$ in hyperbolic lattices, leaving a macroscopic number of removed constraints.

Conclusions and discussions.—In this Letter we generalize Bloch's theorem to high-dimensional irreps of infinite hyperbolic lattices, using linear combinations of Wannier basis. We find that hyperbolic lattices exhibit a number of unusual features, in contrast to Euclidean lattices, from high degeneracy of band structures to modifications of bulk-edge correspondence that require high-dimensional irreps. We apply this theory to a model mechanical hyperbolic lattice, and compute its band structure and zero modes.

The same as Bloch's theorem in Euclidean space, once an irrep is given, our theorem enables us to find all $d^2 \times n$ eigenmodes of this irrep. In parallel to our theorem, another interesting question is to find all irreps of translation groups of hyperbolic lattices, which is a nontrivial mathematical problem due to the rich variety of hyperbolic lattices and the nonabelian nature of their translation groups. In contrast to Euclidean space, where all irreps can be labeled by k points in the BZ, hyberbolic lattices require infinitely many high-dimensional "BZs" (e.g., for lattices studied in Ref. [28], d-dimensional irreps span a $[(2g-2)d^2+2]$-dimensional space).

A number of interesting new questions arise for future studies. For example, how do acoustic phonon branches show up in this formulation, and what is the new form of Goldstone's theorem [29,30]? Interestingly, in the mechanical hyperbolic lattice we considered here, $k=0$ modes in 1D representation and $\lambda=0$ modes in 2D (reducible) representation all have finite frequencies $\omega>0$, in contrast to acoustic phonon modes in Euclidean lattices, which are protected to have $\omega=0$ at $k=0$ by Goldstone's theorem. The reason is that uniform translations in hyperbolic lattices are isometries which can be described as boosts in the hyperboloid model, instead of $k=0$ modes. It would be very interesting to show the new form of Goldstone's theorem. Furthermore, unusual symmetries and bulk-edge correspondence in hyperbolic lattices also provide a huge space for new topological states.

This work was supported in part by the Office of Naval Research (MURI N00014-20-1-2479 N. C., F. S., J. M., K. S., X. M.).

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