

## Systematic generation of Hamiltonian families with dualities

Michel Fruchart,<sup>1,2,\*</sup> Claudia Yao,<sup>1,2</sup> and Vincenzo Vitelli<sup>1,2,3,†</sup>

<sup>1</sup>James Franck Institute, The University of Chicago, Chicago, Illinois 60637, USA

<sup>2</sup>Department of Physics, The University of Chicago, Chicago, Illinois 60637, USA

<sup>3</sup>Kadanoff Center for Theoretical Physics, The University of Chicago, Chicago, Illinois 60637, USA



(Received 22 September 2021; revised 21 November 2021; accepted 9 December 2022; published 15 May 2023)

Dualities are hidden symmetries that map seemingly unrelated physical systems onto each other. The goal of this work is to systematically construct families of Hamiltonians endowed with a given duality and to provide a universal description of Hamiltonian families near self-dual points. We focus on tight-binding models (also known as coupled-mode theories), which provide an effective description of systems composed of coupled harmonic oscillators across physical domains. We start by considering the general case in which group-theoretical arguments suffice to construct families of Hamiltonians with dualities by combining irreducible representations of the duality operation in parameter space and in operator space. When additional constraints due to system-specific features are present, a purely group-theoretic approach is no longer sufficient. To overcome this complication, we reformulate the existence of a duality as a root-finding problem, which is amenable to standard optimization and numerical continuation algorithms. We illustrate the generality of our method by designing concrete toy models of photonic, mechanical, and thermal metamaterials with dualities.

DOI: [10.1103/PhysRevResearch.5.023099](https://doi.org/10.1103/PhysRevResearch.5.023099)

### I. INTRODUCTION

Symmetry groups and their representations are key tools in material and metamaterial design [1–6]. Symmetries and their breaking play a crucial part in determining the properties of a material, including phase transitions [7], band structures, topological phases [8], and physical responses [2,3]. For instance, piezoelectricity or optical activity can only exist in crystals that do not possess a center of inversion [2,3]. But, what is really a symmetry? If we approximate a material as a set of regularly arranged points in space (a crystal), there is an easy answer: Symmetries are all transformations of space such as translations, rotations, reflections (in general, isometries) that leave this set of points invariant. These are spatial symmetries (or more generally, space-time symmetries). To describe a material, we also need to attach to each point some internal degrees of freedom. These could represent, for instance, the amplitude of the electric field, the temperature, the displacement of the particles, or the state of a spin at this point. Spatial symmetries transform these internal degrees of freedom in a definite way, depending on whether they are scalars, vectors, pseudo-vectors, etc. In addition, the system might possess internal symmetries that transform the internal degrees of freedom at each point independently (but leave the system globally invariant). As an example, the Ising model is invariant under the inversion of all spins.

In general, symmetries are transformations that leave the system invariant. This leaves the door open for symmetries that are neither spatial symmetries, nor internal symmetries. Can such hidden symmetries exist? If so, are they just coincidences? To address these questions, it will be helpful to consider families of systems depending on continuous parameters, instead of one system at a time. Accordingly, we consider families of linear operators  $H(p)$  smoothly depending on a parameter  $p$ . The linear operator  $H$  generates the dynamics of the system under consideration, through an equation of motion such as  $i\partial_t\psi = H\psi$  (or a variant, like  $\partial_t^2\psi = H\psi$ ).<sup>1</sup> Here, the vector  $\psi$  describes the state of the system, such as the electromagnetic field in a photonic crystal, the displacements of masses in an elastic network, or the wave function in a quantum system. For convenience, we refer to  $H(p)$  as a (potentially non-Hermitian [9]) Hamiltonian in all cases. We focus on transformations acting linearly on the state  $\psi$ , namely, invertible operators  $U$  mapping  $\psi$  to  $U\psi$ .<sup>2</sup> Symmetries are transformations that commute with the Hamiltonian, i.e., such that  $UHU^{-1} = H$ .

\*fruchart@uchicago.edu

†vitelli@uchicago.edu

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<sup>1</sup>In all the examples we consider, the linear operator  $H$  generates the dynamics of the system, so that its eigenvalues can be related to the frequencies of oscillation or growth rates of the system. This is not required. Identical mathematical manipulations can be performed on linear operators with different mathematical interpretations (e.g., transfer matrices, scattering matrices, matrices of linear coefficients, etc.).

<sup>2</sup>The operators  $U$  are typically assumed to be unitary. This is because unitary operators preserve an inner product  $(\psi, \chi)$ , which is often related to physical quantities (such as a probability amplitude or an energy) that should be unchanged under the action of the symmetry. In addition to linear transformations, one can also consider antilinear transformations.

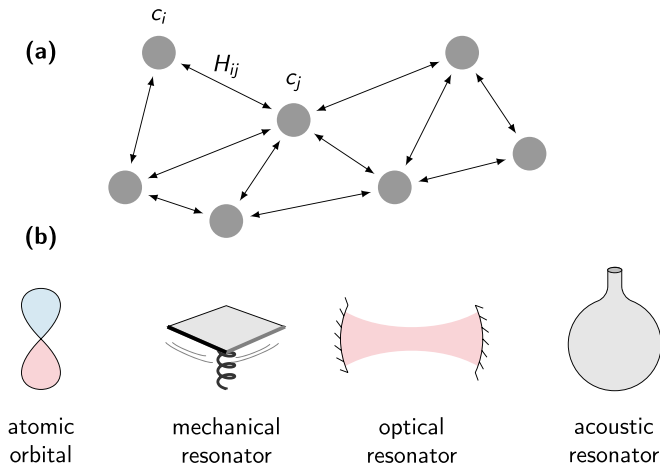


FIG. 1. Effective models. We consider models consisting of coupled resonators  $c_i$  (harmonic oscillators) coupled together with coupling constants  $H_{ij}$ . These can describe, effectively, systems ranging from photonic crystal and phononic crystals to mean-field electrons in the tight-binding approximation.

A duality acts in the same way as a symmetry, but it also changes the parameters in a certain way: It maps a system to another system. Formally, a duality is defined by the combination of a transformation  $U$  (an operator acting on vectors  $\psi$ ) and a smooth function  $f$  defined on the space of parameters  $p$ , such as  $UH(f(p))U^{-1} = H(p)$ . For instance, the properties of a system under a magnetic field  $B$  (playing the role of the parameter  $p$ ) are usually different when the magnetic field is inverted to  $-B$ . Yet, the behaviors of both systems can often be deduced from one another, as exemplified by the Onsager-Casimir relations in nonequilibrium thermodynamics [10]. In this example, the duality is simply embodied in the time-reversal operator  $\Theta$  and the corresponding Hamiltonians  $H(B)$  and  $H(-B)$  are related by  $H(-B) = \Theta H(B)\Theta^{-1}$ . However, the duality operator has no reason to be a simple symmetry, such as a spatial or internal symmetry.

Similar notions of dualities were suggested in systems ranging from self-assembled systems [11] and magnons [12] to quantum rotors [13]. Rich consequences arise when a duality is combined with other constraints such as symmetries or conservation laws, ranging from degeneracies in the band structure [14–16] and topological states [17–20] to symmetries in the phonon response [21] and constraints on the stiffness tensor of an elastic medium [22].

The goal of this paper is to (i) systematically construct families of Hamiltonians endowed with a given duality and (ii) provide a universal description of Hamiltonians families near self-dual points. We are particularly interested in the consequences of dualities on the properties of spatially extended materials (and metamaterials). To handle such systems, we focus on tight-binding models (also known as coupled-mode theories), which describe a collection of coupled harmonic oscillators<sup>3</sup> ranging from atomic orbitals and mechanical res-

<sup>3</sup>As it is an effective description, the oscillators in the tight-binding model might not be directly related to the physical entities composing the system.

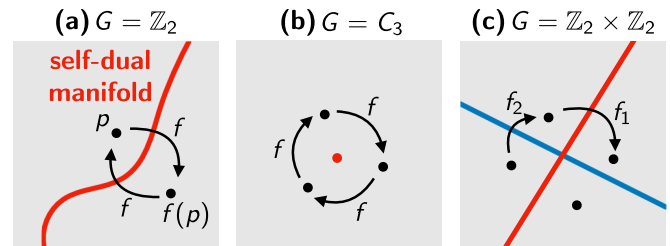


FIG. 2. Examples of duality groups. In (a) and (b), the duality group  $G$  is generated by a single generator, corresponding to the map  $f$ . The self-dual points form a self-dual manifold [a line in (a) and a point in (b)], drawn in red. In (c), the group is generated by two elements corresponding to the maps  $f_1$  and  $f_2$ , each of which has a line of fixed points (drawn in red and blue), that might intersect at a doubly self-dual point. In all cases, the orbit of a typical point  $p$  is shown (black filled circles).

onators to optical cavities, see Fig. 1. These models provide a universal effective description of linear systems. Most crucially from an engineering perspective, systematic methods have been developed to solve the inverse problem of designing realizable systems that correspond to a given tight-binding Hamiltonian [23–29].

Sections II–VI contain definitions and general methods that highlight the formal structure of the theory. For concrete examples across different domains of physics and engineering, the reader can skip to Secs. IV (photonic crystal), V (diffusive thermal metamaterial), and VI C 2 (mechanical metamaterial).

## II. DUALITIES IN CONTINUOUS FAMILIES OF HAMILTONIANS

### A. Introduction

We consider a parameter space  $P$  and call  $\hat{H}(p)$  the Hamiltonian of the system with the parameters  $p \in P$ . The function  $p \mapsto H(p)$ , assumed to be smooth, defines a continuous family of Hamiltonians.

We say that the family of Hamiltonians  $\hat{H}(p)$  is endowed with a duality when

$$\hat{U} \hat{H}(f(p)) \hat{U}^{-1} = \hat{H}(p), \quad (1)$$

where  $\hat{U}$  is an invertible operator and  $f$  is a map from the parameter space  $P$  to itself.<sup>4</sup> We emphasize that the duality is determined not only by  $\hat{U}$  but also by  $f$ . The fixed points of the map  $f$  are called self-dual points (Fig. 2). At a self-dual point,  $\hat{H}(p) \equiv \hat{H}(f(p))$  and the duality reduces to a symmetry. This definition is inspired by similar kinds of dualities crucial in statistical physics [30], mechanics [31,32], condensed matter physics [33–35], or high-energy physics [36,37]. In particular, we refer to Refs. [38,39] for an algebraic approach to dualities.

A duality acts both on parameter space  $P$  via  $f$  and on the Hilbert space of physical states  $\mathcal{H}$  via  $\hat{U}$ . At the level of Eq. (1), the duality acts directly on the space  $\text{End}(\mathcal{H})$  of linear maps on  $\mathcal{H}$ , via the function  $\text{Ad}_{\hat{U}}$  defined by  $\text{Ad}_{\hat{U}}(H) =$

<sup>4</sup>We assume that  $f$  is a homeomorphism: A continuous bijection with a continuous inverse.

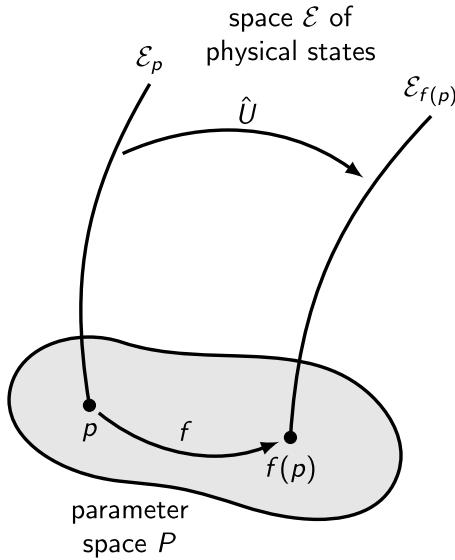


FIG. 3. Dualities and equivariant vector bundles. The space  $\mathcal{E}$  of physical states is described as a vector bundle over parameter space  $P$ . The function  $f$  on parameter space  $P$  is seen as an action of an abstract duality group  $G$ , and the duality operator  $\hat{U}$  as a representation of  $G$  on the vector bundle of physical states. Hence,  $\hat{U}$  maps the fiber  $\mathcal{E}_p$  over a point  $p \in P$  to the fiber  $\mathcal{E}_{f(p)}$  over the point  $f(p)$ .

$UHU^{-1}$ . [The space  $\text{End}(\mathcal{H})$  contains all possible Hamiltonians or dynamical matrices.] Hence, the overall action of a duality is described by the pair  $\mathcal{U} = (f, \text{Ad}_U)$ .

In principle, multiple duality operations can be present [Fig. 2(c)]. Consider two pairs  $\mathcal{U}_1 = (f_1, \text{Ad}_{U_1})$  and  $\mathcal{U}_2 = (f_2, \text{Ad}_{U_2})$  satisfying Eq. (1). Then,  $\mathcal{U}_1\mathcal{U}_2 = (f_1 \circ f_2, \text{Ad}_{U_1} \circ \text{Ad}_{U_2})$  must also satisfy Eq. (1). As both the maps  $f$  and the operators  $\hat{U}$  are invertible, the duality operations have an inverse. Hence, we can see the duality operations  $\mathcal{U}_a$  as the representations of an abstract duality group  $G$  acting on the space  $P \times \mathcal{H}$ , or on  $P \times \text{End}(\mathcal{H})$ . We assume that each duality operation  $\mathcal{U}$  has a finite order  $n$ , such that  $\mathcal{U}^n$  is the identity.<sup>5</sup> In the next section II B, we take a slightly more formal perspective and define dualities starting from this abstract

<sup>5</sup>The order of an operation  $\mathcal{O}$  is the smallest integer  $n$  such that  $\mathcal{O}^n = \text{Id}$  is the identity (the order is set to  $\infty$  when no such integer exists). As a duality  $\mathcal{U}$  is composed of two pieces  $f$  and  $U$ , we can define two separate orders, but we will assume that they are equal, and finite. To be precise, let first  $m$  be the order of the duality map, i.e., the smallest integer such that  $f^{\circ m}(p) = p$  for all  $p$  (here,  $f^{\circ m} = f \circ f \circ \dots \circ f$  is the  $m$ th iterate of the function  $f$ , where  $\circ$  represents composition). Second, let  $n$  be the order of the duality operator, such that  $\text{Ad}_U^n = \text{id}$  (we can define yet another order  $n'$  such that  $U^{n'} = \text{Id}$  is the identity operator, and in general,  $n \neq n'$ , but  $n$  is the relevant quantity). We assume that  $m = n$ , and refer to this integer as *the* order of the duality. When  $m \neq n$ , the Hamiltonian is either endowed with additional symmetries, or there are redundancies in the parameters (i.e., there are equal Hamiltonians for different values of parameters). For simplicity, we do not consider these situations in this work. Besides, we assume that the order  $n = m$  of the duality is finite. This needs not be the case. As a counter-example, consider the function

group. In Sec. III and the rest of the paper, we will focus on the situation in which a single duality operation with finite order  $n$  is present; then,  $G$  is the cyclic group  $C_n$ .

**B. Duality groups and equivariant vector bundles**

In this section (which can safely be skipped), we look at dualities from a slightly more formal point of view summarized in Figs. 2 and 3. Previously, we have implicitly assumed that the space of physical states  $\mathcal{H}$  does not depend on the parameters. In general,  $P \times \mathcal{H}$  may be replaced by an arbitrary vector bundle  $\mathcal{E}$  over the parameter space  $P$ , and  $P \times \text{End}(\mathcal{H})$  may be replaced by the endomorphism bundle  $\text{End}(\mathcal{E})$  (see Refs. [40,41] for introductions to vector bundles). Dualities can then be expressed in terms of equivariant vector bundles, i.e., vector bundles equipped with a notion of symmetry (see Refs. [42–44] and references therein).

We start with an abstract duality group  $G$ . The group elements  $g \in G$  are an abstract version of the different dualities acting on our system; we still have to specify how they act. To do so, we consider an action  $f : G \times P \rightarrow P$  of  $G$  on parameter space. Each  $g \in G$  gives rise to a function  $p \mapsto f_g(p)$  on  $P$ , and these functions compose according to  $G$  (in particular,  $f_g \circ f_h = f_{gh}$  for  $g, h \in G$ ). This specifies how parameters change under the duality  $g$ . Self-dual points of the operation  $g \in G$  are then defined as fixed points of  $f_g$  (see Fig. 2).

Then, we define a linear action  $U : G \times \mathcal{E} \rightarrow \mathcal{E}$  of  $G$  on the vector bundle  $\mathcal{E}$  of physical states (Fig. 3). It specifies how states are transformed. We impose that  $U_g = U(g, \cdot)$  is a linear map from the fiber  $\mathcal{E}_p$  over  $p$  to the fiber  $\mathcal{E}_{f_g(p)}$  over  $f_g(p)$ . This is an equivariance condition, which simply means that a state  $\psi$  of the system with parameters  $p$  is mapped to a state  $U_g\psi$  of the system with parameters  $f_g(p)$ . Hence, we ended up requiring that  $\mathcal{E}$  is a  $G$ -equivariant vector bundle. We can deduce how operators transform from the way states transform. Accordingly, an operator  $H$  acting on the states of the system with parameters  $p$  is mapped to  $U_g H U_g^{-1}$ , which is an operator acting on the states of the system with parameters  $f_g(p)$ . In other words, the endomorphism bundle is then also  $G$ -equivariant with the corresponding adjoint action.

**III. GENERATING DUAL FAMILIES ON DEMAND**

**A. General strategy**

Given a duality operator  $\hat{U}$  (acting on a certain space that is also given), we wish to systematically find the families of Hamiltonians  $p \mapsto \hat{H}(p)$  satisfying

$$\hat{U}\hat{H}(f(p)) = \hat{H}(p)\hat{U}. \tag{2}$$

Ideally, we would like an algorithm whose input is composed of a suitable description of the space of states (e.g., a crystal  $\mathcal{C}$  with its Bravais lattice and unit cell and the internal degrees

$f(p) = p^2$  on the parameter space  $P = [-1, 1]$ , which has infinite order. Similarly, consider the diagonal matrix  $U = \text{diag}(e^{i\alpha}, e^{i\beta})$ . Its action by conjugation on a matrix  $H$  multiplies the off-diagonal elements of  $H$  by  $e^{\pm i(\alpha-\beta)}$  and has infinite order when  $\alpha - \beta$  is irrational.

of freedom attached to each site) and of the duality operator  $\hat{U}$ . Its output should consist of some kind of basis whose elements can be combined to express all the families of Hamiltonians satisfying Eq. (2). Methods and tools performing this task have been developed for spatial symmetries. This is the main idea of the theory of invariants of solid-state physics [45–49], which builds upon the abstract theory of invariants in abstract algebra [50]. This approach originated in the study of semiconductors, but it applies to any linear systems, including photonic and phononic crystals [51,52]. Besides, several works have recently been devoted to expanding and automatizing this procedure using computer algebra systems [53–55]. Here, we extend this method to dualities.

To do so, we focus on functions  $f$  that can smoothly be deformed into isometries by a change of coordinate.<sup>6</sup> Further, we assume that the duality map  $f$  acts as a *linear isometry* on parameter space.<sup>7</sup> Namely, we assume that, after a change of coordinate,  $f(p) = Fp$  in which  $F$  is an orthogonal (or unitary) matrix.<sup>8</sup> It will allow us to use group-theoretical methods to describe the general structure of dualities. These methods are practically advantageous to obtain explicit parameterized forms of Hamiltonian families with dualities. The simplest application of this general strategy is presented in Sec. III A 2. The next paragraphs describe the general case.

In Sec. II, we have introduced an abstract duality group  $G$ . Consider a basis of operators  $\hat{H}_\gamma^\mu \in \text{End}(\mathcal{H})$  that transform under an irreducible representation (irrep)  $\Gamma_\gamma$  of  $G$  (here,  $\mu$  labels the different basis vectors of the fixed irrep  $\Gamma_\gamma$ , while  $\gamma$  labels the different irreps). Hence,

$$\hat{U} \hat{H}_\gamma^\mu \hat{U}^{-1} = [\Gamma_\gamma]_{\mu\mu'} \hat{H}_\gamma^{\mu'}, \quad (3)$$

in which there is an implicit sum over the repeated indices. Under our assumptions, the duality map  $f$  is a linear map  $f(p) = Fp$  in which  $F$  is a matrix acting on parameters.

<sup>6</sup>Namely, we ask that there is another homeomorphism  $g$  such that  $g \circ f \circ g^{-1}$  is an isometry, see Ref. [72].

<sup>7</sup>Because we have assumed the duality to have finite order, we consider only periodic homeomorphisms (homeomorphisms  $f$  such that  $f^{\circ m} = \text{id}$  for a finite integer  $m$ ). (The case of infinite-order dualities is outside of the scope of this work.) This hypothesis, along with that  $f$  is an isometry, gives relatively strong constraints on the duality map. If we are only interested about local (i.e., not global) properties in parameter space, this implies that  $f$  is linear. This can be seen from a series expansion near a self-dual point  $p_0$  as follows. Write  $f(p) = f(p_0 + \delta p) = p_0 + F \delta p + \mathcal{O}(\delta p^2)$  where  $\delta p = p - p_0$ . The matrix  $F$  satisfies  $F^m = \text{Id}$  (because  $f^{\circ m} = \text{id}$ ), and is therefore orthogonal. The case of global properties is considerably more complicated; however, several results exist in simple cases. For instance, all the periodic homeomorphism of the real line  $\mathbb{R}$  or on the closed interval  $[-1, 1]$  are either the identity map  $\text{id}$  or topologically conjugate to the reflection map  $x \mapsto -x$ . We direct the reader to Ref. [98] and references therein for more details.

<sup>8</sup>This is a consequence of the Mazur-Ulam theorem and its generalizations, when applicable, as we have assumed that the duality map is an isometry. We direct the reader to Refs. [99–101] and references therein for more details. This assumption is not as restrictive as it may seem: It turns out that in simple cases, it always holds for dualities of finite order (after change of coordinate).

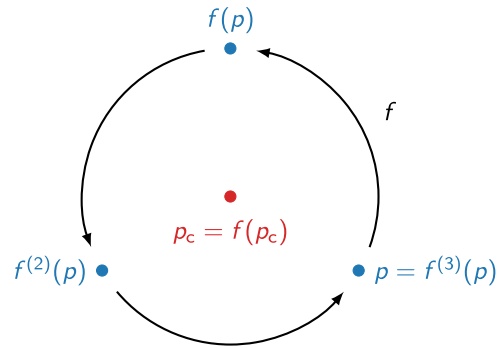


FIG. 4. Action of an order-three duality on parameter space. Here, we consider a duality action  $f$  of order three acting on the 2D plane. We have  $f^{(2)} \neq \text{id}$  and  $f^{(3)} = \text{id}$ . There is a single self-dual point  $p_c$  (in red). A typical point  $p$  (in blue) has an orbit consisting of three points  $p$ ,  $f(p)$ , and  $f^{(2)}(p)$ . Applying the duality action a third time maps back to the original point  $f^{(3)}(p) = p$ .

Therefore, consider similarly a basis of functions on parameter space  $a_\gamma^\mu: P \rightarrow P$  that transform under the conjugate irrep  $\Gamma_\gamma^*$ , namely,

$$a_\gamma^\mu(f(p)) = \overline{[\Gamma_\gamma]_{\mu\mu'}} a_\gamma^{\mu'}(p) \quad (4)$$

in which the overline denotes complex conjugation. Note that the functions  $a_\gamma^\mu$  are not assumed to be linear. We can now combine both ingredients into

$$\hat{H}_\gamma(p) \equiv a_\gamma^\mu(f(p)) \hat{H}_\gamma^\mu. \quad (5)$$

We then find

$$\hat{U} \hat{H}_\gamma(Fp) \hat{U}^{-1} = \hat{H}_\gamma(p) \quad (6)$$

using that the matrix  $\Gamma_\gamma$  is unitary.<sup>9</sup> We can now combine the  $\hat{H}_\gamma$  corresponding to all the irreps  $\Gamma_\gamma$  of  $G$  into

$$\hat{H}(p) \equiv \sum_\gamma \hat{H}_\gamma(p) \quad (7)$$

which is a generic family of functions  $\hat{H}(p)$  that satisfies the duality equation (1) with  $f(p) = Fp$ .

### 1. Cyclic duality group

Up to here, our discussion applies to any finite group  $G$  (and with a few modifications, to any compact group). We now focus on single duality operator with finite order  $n \in \mathbb{N}$ . In this case,  $G$  is the cyclic group  $C_n$  (Fig. 4 shows an example of order  $n = 3$  duality). The irreps of  $C_n$  are one-dimensional and the matrices  $\Gamma_\gamma$  are complex numbers of modulus one,  $\Gamma_m = e^{im2\pi/n}$  with  $m = 1, \dots, n$  (we replace the index  $\gamma$  by  $m$  in this example, and there is no need of the index  $\mu$  as the irreps are one-dimensional). Accordingly, the basis matrices  $\hat{H}_m$  for each irreducible representation are characterized by

$$\hat{U} \hat{H}_m \hat{U}^{-1} = e^{im2\pi/n} \hat{H}_m. \quad (8)$$

<sup>9</sup>We get  $\hat{U} \hat{H}_\gamma(Fp) \hat{U}^{-1} = \delta_{\mu\nu} \overline{[\Gamma_\gamma]_{\mu\mu'}} [\Gamma_\gamma]_{\nu\nu'} a_\gamma^{\mu'}(p) \hat{H}_\gamma^{\nu'}$  and as  $[\Gamma_\gamma]$  is unitary, we have  $\delta_{\mu\nu} \overline{[\Gamma_\gamma]_{\mu\mu'}} [\Gamma_\gamma]_{\nu\nu'} = [[\Gamma_\gamma]^\dagger [\Gamma_\gamma]]_{\mu'\nu'} = \delta_{\mu'\nu'}$  (where  $\dagger$  is the conjugate of the transpose) which gives the result.



(Note that this equation could be rewritten without complex numbers, by pairing elements with conjugate characters.) If the duality operator  $\hat{U}$  was specified, solving Eq. (8) for  $\hat{H}_m$  would produce explicit basis matrices; we will give an example in Sec. III A 2. Following the strategy delineated above, we wish to cancel the phase factor  $e^{im2\pi/n}$  by changing the value of the parameters. To do so, consider the two-component parameter  $p = (p_x, p_y)$  that we represent as the complex number  $z = p_x + ip_y$ . The minimal parameter space is  $P = \mathbb{R}^2 \simeq \mathbb{C}$ , so that we can represent the duality group on  $P$  by considering the function  $f(z) = e^{-i2\pi/n}z$  on  $P$  (and its iterates  $f \circ f$ , etc.). We then consider functions  $z \mapsto a_m(z)$  satisfying

$$a_m(e^{-i2\pi/n}z) = e^{-im2\pi/n}a_m(z). \tag{9}$$

(Again, explicit functions can be constructed, see Sec. III A 2 for an example.) Then, the combinations

$$\hat{H}(z) = \sum_m a_m(z)\hat{H}_m \tag{10}$$

satisfy the duality relation

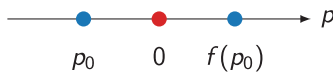
$$\hat{U}\hat{H}(e^{-i2\pi/n}z)\hat{U} = \hat{H}(z). \tag{11}$$

**2. Example: The group  $\mathbb{Z}_2$**

In this section, we describe in detail a concrete example in the most simple situation where  $G = C_2 \equiv \mathbb{Z}_2$ . We wish to obtain the families of Hamiltonians  $\hat{H}(p)$  satisfying

$$\hat{U}\hat{H}(-p)\hat{U}^{-1} = \hat{H}(p). \tag{12}$$

Here,  $f(p) = -p$  and the 1D parameter space is  $P = [-1, 1]$  (or  $\mathbb{R}$ ). Hence,  $f$  can be seen as a representation of the group  $\mathbb{Z}_2$  on parameter space. There is a single self-dual point  $p = 0$  (in red).



Consider arbitrary self-dual and anti-self-dual matrices  $\hat{H}_\pm$  satisfying

$$\hat{U}\hat{H}_\pm\hat{U}^{-1} = \pm\hat{H}_\pm \tag{13}$$

and arbitrary odd and even functions  $a_\pm$  on parameter space, satisfying

$$a_\pm(-p) = \pm a_\pm(p). \tag{14}$$

These correspond to the two irreducible representations (odd and even) of  $\mathbb{Z}_2$ . Then, the combinations

$$a_+(p)\hat{H}_+ \text{ and } a_-(p)\hat{H}_- \tag{15}$$

satisfy the duality relation. The sum of any of such combinations (with arbitrary prefactors) also satisfies the duality. Hence, we consider a basis  $\hat{H}_\pm^i$  of linearly independent solutions of Eq. (13) and arbitrary functions  $a_\pm^i(p)$  satisfying Eq. (14) to obtain a general family of Hamiltonians with duality

$$\hat{H}(p) = \sum_i a_+^i(p)\hat{H}_+^i + \sum_i a_-^i(p)\hat{H}_-^i. \tag{16}$$

To go further, we must specify the duality operator. Let us choose, as an example,

$$\hat{U} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{17}$$

as the duality operator. Solving Eq. (13), we find two self-dual basis matrices

$$H_+^1 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad H_+^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{18}$$

and two anti-self-dual ones:

$$H_-^1 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad H_-^2 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \tag{19}$$

Then, we look for functions satisfying Eq. (14). As an example,<sup>10</sup> let us consider polynomials with only even or odd powers of  $p$ , namely,

$$a_+^i(p) = \sum_n \alpha_n^i p^{2n} \tag{20}$$

and

$$a_-^i(p) = \sum_n \beta_n^i p^{2n+1}, \tag{21}$$

in which  $\alpha_n^i$  and  $\beta_n^i$  are arbitrary coefficients and  $i = 1, 2$ .

Finally, we combine everything together to write

$$H(p) = \sum_{i=1,2} \sum_{\eta=\pm} a_\eta^i(p)H_\eta^i, \tag{22}$$

which is a family of Hamiltonians with the desired duality.

**B. Spatially periodic metamaterials**

**1. General considerations**

We now focus on spatially periodic systems (crystals) which are obtained by repeating a unit cell over a Bravais lattice  $\Gamma$  (see Appendix A and references therein for details). To do so, we consider Hamiltonians of the form

$$\hat{H}(p) = \sum_{\gamma \in \Gamma} h(\gamma, p)\hat{T}(\gamma) \tag{23}$$

in which  $\hat{T}(\gamma)$  is the translation operator by a Bravais lattice vector  $\gamma$ ,  $h(\gamma)$  is a finite-dimensional matrix acting on the degrees of freedom in the unit cell. The translation operator acts on functions  $\psi$  as  $[\hat{T}(\gamma)\psi](x) = \psi(x - \gamma)$  for all points  $x$  of the crystal.<sup>11</sup> All translation invariant Hamiltonians can be

<sup>10</sup>As another example, in the case of  $P = [-1, 1]$ , we can also take for  $a_\pm^i$  a sum of Chebyshev polynomials  $T_n$  with even (odd) order  $n$ , as that satisfy  $T_n(-p) = (-1)^n T_n(p)$  ( $n \in \mathbb{N}$ ), as Chebyshev polynomials are orthogonal to each other.

<sup>11</sup>To make contact with equivalent notations, note that the translation operator can be written  $\hat{T}(\gamma) = \sum_{x \in \mathcal{C}} |x + \gamma\rangle\langle x|$  or equivalently  $\hat{T}(\gamma) = \sum_{x \in \mathcal{C}} \hat{c}_{x+\gamma}^\dagger \hat{c}_x$  where  $|x\rangle$  is a state fully localized at the point  $x$  of the crystal, and  $\hat{c}_x^{(\dagger)}$  the corresponding annihilation (creation) operator. Given a basis  $|e_i\rangle$  of the Hilbert space of the degrees of freedom in the unit cell, we can further decompose  $h(\gamma, p) = \sum h_{ij}(\gamma, p)|e_i\rangle\langle e_j|$  in which the matrix elements  $h_{ij}(\gamma, p)$  are now scalars. The Hamiltonians  $\hat{H}(p)$  act on the Hilbert space spanned by states of the form  $|x\rangle \otimes |e_i\rangle$ .

written in this form. For convenience, we also assume that the connections between the oscillators have a finite range (this hypothesis is not crucial, but simplifies the manipulations). Correspondingly, the sum in Eq. (23) is restricted to a finite subset  $\Gamma_0 \subset \Gamma$  of the Bravais lattice  $\Gamma$ , centered at the origin.

We also decompose the duality operator as

$$\hat{U} = \sum_{\gamma, \gamma' \in \Gamma} u(\gamma, \gamma') |\gamma\rangle \langle \gamma'| \quad (24)$$

in which  $u(\gamma, \gamma')$  are again finite-dimensional matrices, and in which  $|\gamma\rangle$  represents the function in  $\ell^2(\Gamma)$  having value one at  $\gamma$  and zero elsewhere.<sup>12</sup>

Equation (2) can be decomposed over the translation operators and transformed to a finite number of linear relations between the matrix elements  $h_{ij}(\gamma, p)$  and the dual matrix elements  $h_{ij}(\gamma, f(p))$ , gathered in a linear equation of the form

$$\mathcal{A}[\hat{U}] \vec{h}(p) = \mathcal{B}[\hat{U}] \vec{h}(f(p)) \quad (26)$$

in which the matrix elements  $h_{ij}(\gamma, p)$  are all gathered in the vector  $\vec{h}(p)$ , etc. and in which  $\mathcal{A}[\hat{U}]$  and  $\mathcal{B}[\hat{U}]$  are known matrices (that depend on the duality operator).<sup>13</sup> Equation (26) can be solved (numerically or symbolically, see, e.g., Refs. [56,57]), giving  $\vec{h}(f(p))$  as a function of  $\vec{h}(p)$  (or conversely).

In practice, it is convenient to obtain explicit parameterized forms of the Hamiltonian families. To do so, we restrict our attention to dualities in which the duality map  $f$  is linear (as well as all dualities that can be obtained from those by reparameterization). This hypothesis allows us to use the structure described in Sec. III A to obtain a systematic way of explicitly constructing the families of Hamiltonians with a duality.<sup>14</sup> We first make change of variables to make parameter space as symmetric as possible (we assume that the duality map  $f$  becomes an isometry); second, we need to use a basis of functions adapted to the symmetry. We can then specialize the strategy of Sec. III A to Eq. (26). To get an explicit form, one might further parametrize these functions, e.g., through a series expansion, a Fourier or Chebyshev decomposition, etc.

## 2. Bloch representation

In spatially periodic systems, it is convenient to use the Bloch (momentum space) representation. We refer to Ap-

<sup>12</sup>We can also write more explicitly

$$\hat{U} = \sum_{\substack{\gamma, \gamma' \in \Gamma \\ \xi, \xi' \in \mathcal{F}}} u_{\xi', \xi}(\gamma', \gamma) |\gamma', \xi'\rangle \langle \gamma, \xi|, \quad (25)$$

in which  $|\gamma, \xi\rangle$  are a basis of  $\ell^2(\mathcal{C})$  of functions  $x \mapsto \delta(x - (\gamma + \xi))$  (for  $\gamma \in \Gamma$  and  $\xi \in \mathcal{F}$ , where  $\mathcal{F}$  is a fundamental domain) having value one at  $\gamma + \xi \in \mathcal{C}$  and zero elsewhere.

<sup>13</sup>One can further convert Eq. (26) into the homogeneous linear system  $[\mathcal{A}, \mathcal{B}][\vec{h}(p), \vec{h}(f(p))]^T = 0$ . The vectors and matrices are finite, provided that we restrict the model to have finite range connections (corresponding to the restriction to  $\Gamma_0$ ).

<sup>14</sup>It is still possible to directly solve the duality equation when  $f$  is nonlinear, but we do not have a systematic way of writing an explicit parametrization.

pendix A for details. In short, each Hamiltonian operator  $\hat{H}(p)$  (for a fixed  $p$ ) is mapped to a continuous family of matrices  $k \mapsto H(p, k)$  with the quasimomentum  $k$  in the Brillouin zone (a torus  $T^d$ ). We emphasize that the quasimomentum  $k$  does not play the same role as the external parameter  $p$ : The entire family  $k \mapsto H(k)$  for  $k$  in the Brillouin zone describes a single physical system, while different values of  $p$  correspond to different physical systems. In general, the duality changes the quasimomentum  $k$  to  $\mathcal{O}k$ , in which  $\mathcal{O}$  is an orthogonal matrix. We can then write the equivalent of Eq. (1) for the Bloch Hamiltonians<sup>15</sup>

$$U(\mathcal{O}k) H(f(p), \mathcal{O}k) U^{-1}(\mathcal{O}k) = H(p, k). \quad (27)$$

## 3. Example: Duality in a 1D crystal

Consider a 1D crystal with two degrees of freedom per unit cell, and the duality defined in Bloch space by  $f(p) = -p$ ,  $\mathcal{O}k = -k$  in Eq. (27), as well as

$$U(k) = i\sigma_y = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (28)$$

(Here,  $k \in S^1$  is the one-dimensional quasimomentum.)

In real space, this corresponds to the operator

$$\hat{U} = i\sigma_y \sum_{\gamma} |T(-\gamma)\rangle \langle T(\gamma)| \quad (29)$$

The second part is due to the action  $\mathcal{O}k = -k$  on momentum space.

We now consider Bloch Hamiltonians of the form

$$H(p, k) = H^{(0)}(p) + H^{(1)}(p)e^{-ik} + H^{(-1)}(p)e^{ik}. \quad (30)$$

The duality condition Eq. (27) applied to Eq. (30) gives

$$UH^{(0)}(-p)U^{-1} = H^{(0)}(p), \quad (31a)$$

$$UH^{(1)}(-p)U^{-1} = H^{(-1)}(p), \quad (31b)$$

in which  $U \equiv U(k)$  is defined in Eq. (28).

To handle Eq. (31a), let us follow Sec. III A 2 and look for a basis  $H_{\pm}^i$  of (anti-)self-dual solutions to  $UH_{\pm}^i U^{-1} = \pm H_{\pm}^i$ . As shown in Sec. III A 2,  $H^{(0)}(p)$  is given by the right-hand side (RHS) of Eq. (16). To satisfy Eq. (31b), we can simply take the matrix elements  $H_{ij}^{(1)}(p)$  to be arbitrary smooth functions (without any constraint), and Eq. (31b) then fully determines  $H^{(-1)}(p)$  as a function of  $H^{(1)}(-p)$ .

Let us add an additional specification: We now want  $H(p)$  to be Hermitian. This requires

$$H^{(0)} = [H^{(0)}]^{\dagger} \quad \text{and} \quad H^{(1)}(p) = [H^{(-1)}(p)]^{\dagger}. \quad (32)$$

in addition to Eqs. (31a) and (31b).

Let us first worry about  $H^{(0)}$ . We can first impose the constraint Eq. (31a) as explained above. As the generators  $H_{\pm}^a$  in Eqs. (18-19) are Hermitian, the Hermiticity of  $H^{(0)}$  is then ensured by taking the coefficients  $\alpha_n^i \in \mathbb{R}$  and  $\beta_n^i \in \mathbb{R}$  in Eq. (16). The second condition requires a bit more work: We

<sup>15</sup>We have shortened to  $U(\mathcal{O}k)$  the momentum-dependent duality operator  $U(k, \mathcal{O}k)$ . This is a choice: We could have called the same quantity  $U(k)$ .

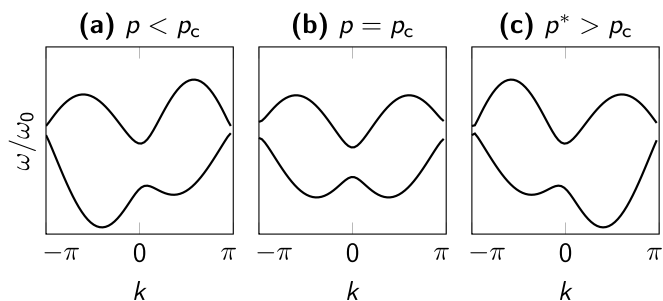


FIG. 5. A duality with no degeneracy. We have used a random polynomial of order 2 [e.g., by taking random coefficients  $\alpha_n^i$  and  $\beta_n^i$  in Eq. (16)]. In this example, there is no bosonic TRI and therefore no degeneracy. Nevertheless, the band structures at dual parameters in (a) and (c) are related by  $k \rightarrow -k$ , while the band structure at the self-dual point is symmetric under this transformation.

are not anymore free to choose an arbitrary function  $H^{(1)}(p)$ . Instead, we have to find all families of matrices satisfying

$$UH^{(1)}(-p)U^{-1} = [H^{(1)}(p)]^\dagger \quad (33)$$

and then set  $H^{(-1)}(p) = [H^{(1)}(p)]^\dagger$ . Proceeding in a similar fashion as in Sec. III A 2, we look for a basis  $\mathcal{B}_\pm = (H_\pm^j)_j$  of the vector spaces of matrices  $H_\pm$  satisfying

$$UH_\pm U^{-1} = \pm [H_\pm(p)]^\dagger. \quad (34)$$

(Note that these  $H_\pm^j$  are not the same as the ones in Sec. III A 2.) We find  $\mathcal{B}_+ = (\sigma_0, i\sigma_1, \sigma_2, i\sigma_3)$  and  $\mathcal{B}_- = (i\sigma_0, \sigma_1, i\sigma_2, \sigma_3)$ , where  $\sigma_j$  are Pauli matrices. These matrices are then combined with odd/even polynomials (with real coefficients) to construct  $H^{(1)}(p)$ .

Putting everything together, we obtain Hermitian Hamiltonians Eq. (30) satisfying the duality condition Eq. (27) with the duality operator defined by Eq. (28). In Fig. 5, we show the band structure of one of these Hamiltonians, chosen at random. (The code used to produce this figure, as well as other results in this paper, is available in Ref. [58].) In this figure, we note that (i) the band structures of dual systems (a) and (c) are obtained by applying the transformation  $k \rightarrow -k$  and (ii) the self-dual band structure is symmetric under  $k \rightarrow -k$ . As we shall see in the next paragraph, richer consequences arise when the duality is combined with other constraints.

### C. Examples in 1D and 3D

We now show the results of the procedure described in Secs. III A and III B. Before, we must make a few choices: What duality operator  $\hat{U}$ , what parameter space  $P$ , and what duality map  $f$  shall we impose? We are free to choose any unitary  $\hat{U}$  and any homeomorphism  $f$ .<sup>16</sup> The most simple dualities are associated with a one-dimensional parameter space  $P = \mathbb{R}$  and  $f(p) = -p$ . We will restrict our attention to this case. We would also like to find a duality operator  $\hat{U}$  as simple as possible, but we ask that the antiunitary operator  $\hat{A} = \hat{U}\mathcal{K}$  (obtained by combining the duality operator  $\hat{U}$  with complex conjugation  $\mathcal{K}$ ) squares to  $\hat{A}^2 = -1$ . In this paragraph,

<sup>16</sup>This is contingent on the existence of free will. We refer to Refs. [102–104] for discussions.

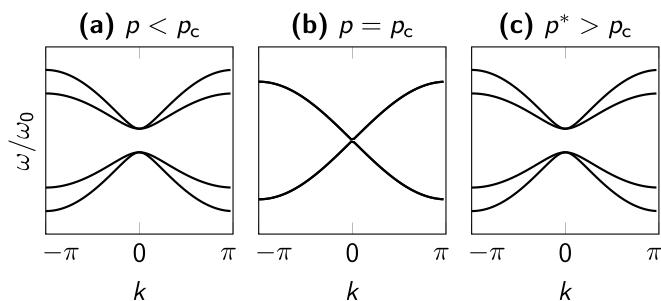


FIG. 6. A one-dimensional example of duality. A  $4 \times 4$  example in 1D. The systems (a) and (c) are dual to each other, while the system (b) is self-dual. The Hamiltonians  $H(p)$  in the family are endowed with the duality in Eq. (35) and with bosonic TRI (the physical space Hamiltonians are real-valued). The coefficients of the Hamiltonian are chosen in order to have a Dirac cone at  $k = 0$ . Because of the combination of the self-duality with bosonic TRI, the spectrum (b) is twofold degenerate.

we constrain all tight-binding Hamiltonians to be real-valued (equivalently, they commute with  $\mathcal{K}$ ). These requirements guarantee (through Kramers theorem, see Appendix C) that the spectra of self-dual Hamiltonians are twofold degenerate everywhere in the Brillouin zone.

This leads us to consider the duality transformation

$$\hat{U} = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y T(a_1) \end{pmatrix} \hat{\mathcal{X}}, \quad (35)$$

in which

$$\hat{\mathcal{X}} = \sum_\gamma |\gamma\rangle\langle\gamma|. \quad (36)$$

In momentum space, this corresponds to Eq. (27) with

$$U(k) = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y e^{-ik \cdot a_1} \end{pmatrix} \quad \text{and} \quad g(k) = -k. \quad (37)$$

As we have seen in the previous example (Sec. III B 3 and Fig. 5), it is possible to obtain families of Hamiltonians (with dualities) that have no striking feature: The bands are typically disconnected from each other. When additional constraints are imposed, the self-duality can lead to additional degeneracies in the band structure. We illustrate this feature in Fig. 6 for a 1D system and in Fig. 7 for a 3D system. In the next sections, we illustrate our procedure in the concrete examples of optical and thermal metamaterials.

## IV. EXAMPLE: DUALITIES IN OPTICAL METAMATERIALS

In this section, we illustrate the generation of a family of metamaterials with a duality in the case of photonic crystals. Consider a planar collection of cylindrical resonators coupled through evanescent waves (Fig. 8). These can be for instance holes in a dielectric slab, laser-written waveguides in a fused silica substrate [25,59], or coupled polariton micropillars [60]. Because of its cylindrical symmetry, each resonator has two degenerate vectorlike modes  $p_x$  and  $p_y$  [see panel (a) of the figure]. For concreteness, let us consider Hermite-Gaussian modes  $H_{10}$  and  $H_{01}$ , and call their common natural frequency

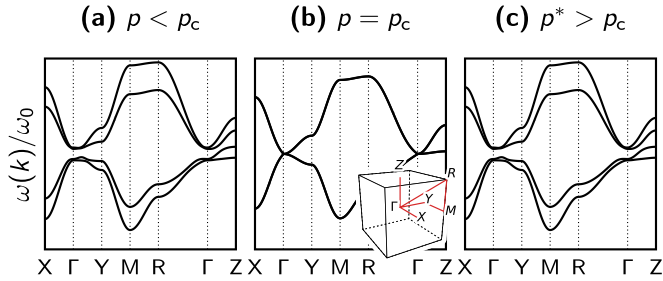


FIG. 7. A three-dimensional example of duality. A  $4 \times 4$  example in 3D. The systems (a) and (c) are dual to each other, while the system (b) is self-dual. We consider a 3D cubic lattice with four degrees of freedom per unit cell. Each unit cell is coupled to the six nearest unit cells with an initially arbitrary  $4 \times 4$  hopping matrix. The duality constraint is then applied. In addition, the coefficients of the Hamiltonian are chosen in order to have a degeneracy at  $k = 0$ . The Hamiltonians  $H(p)$  in the family are endowed with the duality in Eq. (35) and with bosonic TRI (the physical space Hamiltonians are real-valued). Because of the combination of the self-duality with bosonic TRI, the spectrum (b) is twofold degenerate.

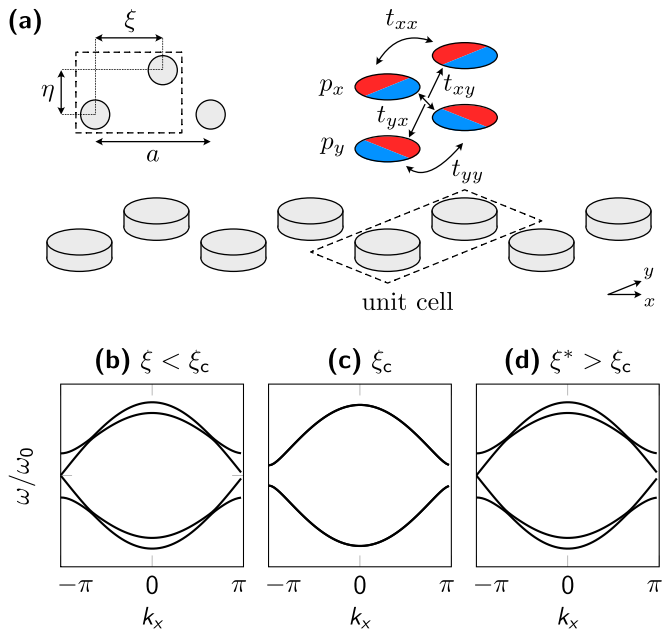


FIG. 8. Photonic metamaterial and its band structure. A 1D photonic metamaterial composed of resonators with a duality. (a) Geometry of the system. Resonators with cylindrical symmetry are arranged in the plane as a horizontal 1D chain resembling a SSH chain. A unit cell (dashed rectangle) is composed of two resonators. The (horizontal) size of the unit cell is  $a$ . The two cylinders in the unit cell are separated by a horizontal distance  $\xi$  and a vertical distance  $\eta$ . We focus on the  $p_x$  and  $p_y$  modes of the resonators (for instance, the Hermite-Gaussian modes  $H_{10}$  and  $H_{01}$ ), that form a vectorial mode  $\vec{p} = (p_x, p_y)$ . For an isolated cylinder, the  $p_x$  and  $p_y$  modes are degenerate because of the rotation symmetry. Because of the geometry, the  $p_x$  modes on one site can couple to both the  $p_x$  and  $p_y$  modes on another site. Representative band structures of the system are plotted in (b-d) as a function of the momentum  $k_x$ . The systems in (b) and (d) are dual, and have identical band structures. The system in (c) is self-dual and has a twofold degenerate band structure. We have set  $a = 1$ ,  $\eta = 1/2$  and (b)  $\xi = 0.2$ , (c)  $\xi = \xi_c \equiv 1/2$ , (d)  $\xi = 0.8$ .

$\omega_0$  (similar results would be obtained for other shapes with the same symmetries). Each resonator  $n$  located at point  $r_n$  has then two modes  $a_n^+(r) = H_{10}(r - r_n)$  and  $a_n^-(r) = H_{01}(r - r_n)$ . The amplitude of the coupling between two resonator modes  $i = (a, n)$ , where  $a = \pm$  labels the two modes on each resonator, is determined by the overlap

$$t_{ij} = \int a_i(r) a_j(r) d^2r \quad (38)$$

between the modes  $a_i$  and  $a_j$ , which can be computed explicitly (see Ref. [58]). This allows us to obtain an effective Hamiltonian

$$H_{ij} = \omega_0 \delta_{ij} + t_{ij} \quad (39)$$

for the  $p_x$  and  $p_y$  modes, that we assume are well-separated from other ( $s$ -like and  $d$ -like) modes in frequency. The amplitudes  $\alpha_i$  of the modes  $a_i$  then evolve according to the equation [25,61–63]

$$i\partial_t \alpha_i = H_{ij} \alpha_j. \quad (40)$$

As an example, consider a one-dimensional chain where the resonators are arranged in a zig-zag configuration (panel a in Fig. 8). There are two resonators per unit cell, located at positions  $(na, 0)$  and  $(na + \xi, \eta)$ , where  $n = 1, 2, \dots$  is the index of the unit cell,  $a$  is the lattice spacing,  $\xi$  and  $\eta$  are parameters. A version of this system has been implemented with coupled semiconductor micropillars in the context of topological lasing [60]. In the basis  $(a_0^+, a_0^-, a_\xi^+, a_\xi^-)$ , where we have labeled by 0 and  $\xi$  the two resonators in one unit cell, the Bloch Hamiltonian reads

$$H(k_x) = \omega_0 \text{Id} + \begin{pmatrix} 0 & M(k_x) \\ M^\dagger(k_x) & 0 \end{pmatrix} \quad (41)$$

in which  $\text{Id}$  is the  $4 \times 4$  identity matrix and

$$M = \begin{pmatrix} 2A + B + 2B\xi - (A + B)\xi^2 & B\eta - (A + B)\eta\xi \\ B\eta - (A + B)\eta\xi & (A + B)(2 - \eta^2) \end{pmatrix},$$

where  $A = e^{-[\eta^2 + \xi^2]/4}$  and  $B = e^{-[\eta^2 + (1 - \xi)^2]/4 + ik_x}$ . When  $\eta = a/2$ , we find that a self-dual point occurs when the system is invariant under mirror reflection, at  $\xi_c = a/2$  [(panel (c))], while the points  $\xi = a/2 - \delta\xi$  and  $\xi^* = a/2 + \delta\xi$  are dual to each other [panels (b) and (d) in Fig. 8]. In this simple example, the two degenerate bands at the self-dual point are completely decoupled, because at this point, the  $p_x$  and  $p_y$  modes on neighboring sites are orthogonal to each other.

## V. EXAMPLE: DUALITIES IN THERMAL METAMATERIAL

In the previous section, we have considered the example of dualities in light waves. However, dualities are not limited to linear waves, they also include other linear systems such as diffusive systems. To illustrate this, we now consider a class of discrete thermal metamaterial described and experimentally realized in Refs. [64–70]. The system consists of pieces of thermally conductive materials (thermal resonators) coupled together by thermal junctions, see Fig. 9. When the coupling is weak enough, each thermal resonator  $i$  can be described with a single temperature  $T_i(t)$ . For instance, Ref. [64] uses nylon rings thermally coupled by grease layers, while Ref. [70] uses



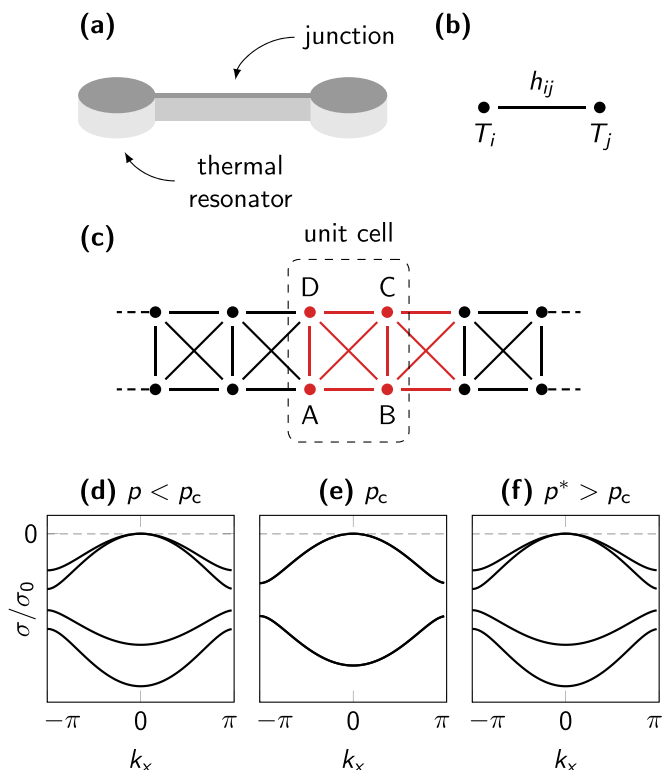


FIG. 9. Thermal metamaterial and its band structure. (a) Schematic of thermal resonators connected by a thermal junction and (b) the corresponding tight-binding graph, in which nodes represent resonators with temperature  $T_i$  and edges represent thermal couplings  $h_{ij}$ . (c) One-dimensional thermal metamaterial. The unit cell is highlighted in red. [(d)–(f)] Band structure of the thermal metamaterials. The eigenvalues are of the form  $s(k_x) = \sigma(k_x) + i\omega(k_x)$ . Here, the frequencies  $\omega(k_x) = 0$  vanish, so we plot only the growth rate  $\sigma(k_x)/\sigma_0$ , in which  $\sigma_0$  is an inverse time scale. The systems in (d) and (f) are dual to each other, and the system in (e) is self-dual. We have set  $h_{AC} = 4$ ,  $h_{AB} = p - 1$ ,  $h_{AD} = -p$ ,  $g_{CD} = -1$ ,  $g_{AC} = 5 - p$ ,  $g_{AB} = 1$ ,  $h_{BC} = -p$ ,  $g_{BD} = p + 5$ ,  $h_{BD} = 4$ ,  $h_{CD} = p + 1$  and (d)  $p = -1$ , (e)  $p = 0$ , (f)  $p = -1$ .

aluminium disks connected by narrow aluminium channels. The heat current between two resonators  $i$  and  $j$  is  $J_{ij} = h_{ij}(T_j - T_i)$ , in which  $h_{ij}$  measures the rate of heat exchange. The transport of heat in a collection of resonators  $i$  is then described by the equation

$$\partial_t T_i = \sum_j h_{ij}(T_j - T_i). \quad (42)$$

In a passive system,  $h_{ij} = h_{ji} \geq 0$ . These constraints can be lifted in active systems. For instance, both negative  $h_{ij}$  and  $h_{ij} \neq h_{ji}$  could be achieved using temperature sensors, heaters, and a Peltier heat pump.

We consider a one-dimensional crystal containing four resonators per unit cell, as represented in Fig. 9(c). We label the resonators by  $i = (a, n)$  in which  $a = A, B, C, D$  labels the inequivalent resonators and  $n \in \mathbb{Z}$  the position in the 1D Bravais lattice. The connections internal to the unit cell are labeled  $h_{ab} = h_{ba}$  and the connections from one unit cell to the next one are labeled  $g_{ab} = g_{ba}$  ( $a, b = A, B, C, D$ ). We have assumed that the junctions are reciprocal for simplicity.

The linear operator describing this system is

$$\hat{H} = \begin{pmatrix} \tilde{D}_A & h_{AB} & h_{AC} & h_{AD} \\ h_{AB} & \tilde{D}_B & h_{BC} & h_{BD} \\ h_{AC} & h_{BC} & \tilde{D}_C & h_{CD} \\ h_{AD} & h_{BD} & h_{CD} & \tilde{D}_D \end{pmatrix} + \begin{pmatrix} 0 & g_{AB}\hat{T}_1 & g_{AC}\hat{T}_1 & 0 \\ g_{AB}\hat{T}_{-1} & 0 & 0 & g_{BD}\hat{T}_1 \\ g_{AC}\hat{T}_{-1} & 0 & 0 & g_{CD}\hat{T}_1 \\ 0 & g_{BD}\hat{T}_{-1} & g_{CD}\hat{T}_{-1} & 0 \end{pmatrix}, \quad (43)$$

in which we have defined

$$\tilde{D}_A = -g_{AB} - g_{AC} - h_{AB} - h_{AC} - h_{AD}, \quad (44a)$$

$$\tilde{D}_B = -g_{AB} - g_{BD} - h_{AB} - h_{BC} - h_{BD}, \quad (44b)$$

$$\tilde{D}_C = -g_{AC} - g_{CD} - h_{AC} - h_{BC} - h_{CD}, \quad (44c)$$

$$\tilde{D}_D = -g_{BD} - g_{CD} - h_{AD} - h_{BD} - h_{CD}. \quad (44d)$$

The eigenvalues  $s = \sigma + i\omega$  of  $\hat{H}$  are composed of a growth/decay rate  $\sigma$  and a frequency  $\omega$ .

We consider the duality operator

$$\hat{U} = \sigma_1 \otimes (i\sigma_2) = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad (45)$$

in which  $\sigma_i$  are Pauli matrices. Following the method of Sec. III, we find that a self-dual system occurs provided that the following conditions are satisfied:

$$h_{AC} = h_{BD}, \quad g_{AC} = g_{BD}, \quad h_{BC} = h_{AD} = 0, \quad (46a)$$

$$h_{AB} = g_{CD} = -h_{CD} = -g_{AB}. \quad (46b)$$

In passive systems where couplings must be non-negative, the conditions Eq. (46b) should be replaced with  $h_{AB} = h_{CD} = g_{CD} = g_{AB} = 0$ . In this case, Eq. (43) becomes block-diagonal and describes two disconnected chains. When negative couplings are allowed, however, self-dual systems can not always be decomposed into two disconnected subsystems.<sup>17</sup> Similarly, an anti-self-dual system occurs

<sup>17</sup>In the example of Fig. 9, we have considered active thermal metamaterials in which energy can be injected in the system from the outside. We have chosen the parameters so that the eigenvalues (growth rates) are nonpositive, so that the system is stable. In the general case, positive growth rates can occur: In this case, we have to analyze the system beyond the linear approximation. This raises the more general question of whether dualities can be extended to nonlinear dynamical systems. They indeed can. First, consider a dynamical system depending on a set of parameters  $p$ . It can be modelled by a differential equation of the form  $\partial_t X = F(X, p)$ , in which  $X$  is a vector representing the state of the system, and  $F$  is a (possibly nonlinear) function defining the dynamical system. Definition (1) of a duality can then be extended as

$$F(\hat{U}X, p) = \hat{U}F(X, f(p)). \quad (47)$$

When  $f$  is the identity map, this equation defines an equivariant dynamical system [72,105,106]. In the general case, Eq. (47) defines dualities in general dynamical systems.

when

$$h_{AD} = h_{BC}, \quad h_{AB} = h_{CD}, \quad (48a)$$

$$h_{AC} = -h_{BD}, \quad g_{AC} = -g_{BD}, \quad (48b)$$

$$g_{AB} = g_{CD} = -h_{BC} - h_{CD}. \quad (48c)$$

We can then obtain a family of systems with a duality by combining a self-dual linear operator and an anti-self-dual linear operator (see Sec. III A 2). A numerical example is given in the caption of Fig. 9, in which we plot the corresponding band structures for a pair of dual configurations (d) and (f), as well as for a self-dual configuration (e).

## VI. DUALITIES IN CONSTRAINED LINEAR SYSTEMS

In the previous sections, we have assumed that all tight-binding Hamiltonians are available to us, perhaps up to some linear constraints such as asking for Hermitian or real-valued Hamiltonians. In particular, we have heavily relied on the hypothesis that linear combinations of physically relevant Hamiltonians are still physically relevant Hamiltonians. This is not always the case. As an example, consider the dynamical matrix  $\hat{D}$  describing the vibrations of a set of massive particles arranged on a  $d$ -dimensional crystal and ruled by Newton equations

$$\partial_t^2 \phi = -\hat{D}\phi, \quad (49)$$

in which  $\phi$  are the displacements of the masses with respect to their equilibrium positions (see Sec. VIC below for details). Even though the dynamical matrices  $\hat{D}_1$  and  $\hat{D}_2$  might describe two perfectly reasonable networks of particles connected by springs, there is no reason why  $\hat{D}_1 + \hat{D}_2$  should necessarily describe yet another networks of spring-connected particles.<sup>18</sup> More generally, one might want to consider systems in which only a certain portion of parameter space is accessible, either for fundamental or for practical reasons. The purpose of this section is to tackle the analysis of dualities in this class of systems.

Deprived from the powerful tools of linear algebra and group theory, we are left with no other choice than to resort to numerical analysis. To do so, we start by reformulating the duality condition (1) as an optimization problem. First, we define

$$\mathcal{F}(p, p') = \hat{U} \hat{H}(p') \hat{U}^{-1} - \hat{H}(p), \quad (50)$$

which is a function defined on the doubled parameter space  $P \times P$ . Indeed, Eq. (1) is satisfied whenever

$$\mathcal{F}(p, f(p)) = 0. \quad (51)$$

We define  $s = (p, p')$  and interpret  $\mathcal{F}(s) \equiv \mathcal{F}(p, p')$  as a vector composed of all its matrix elements.<sup>19</sup> Conversely, any

<sup>18</sup>It is even dubious that the notation  $\hat{D}_1 + \hat{D}_2$  has a well-defined meaning, because  $\hat{D}_1$  and  $\hat{D}_2$  act on different spaces, the spaces of infinitesimal deformations about different configurations.

<sup>19</sup>In practice, it is convenient to focus on the cases in which there is a finite number of translation operators in Eq. (50) [see the discussion

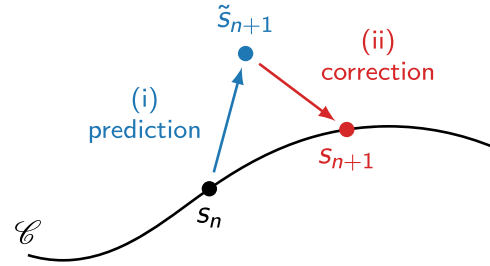


FIG. 10. Numerical continuation. Let us assume that the solutions of the equation  $F(s) = 0$  form a curve  $\mathcal{C}$ . Starting from a point  $s_0$  in this curve [so  $F(s_0) = 0$ ], we want to find the whole curve. This is the job of numerical continuation (or numerical path following) algorithms. The main idea consists in combining (i) a prediction step (in blue) that starts from a point  $s_n$  on the curve to suggest a new point  $\tilde{s}_{n+1}$  that is a bit off the curve, but in the good direction with (ii) a correction step (in red) that projects  $\tilde{s}_{n+1}$  to a new point  $p_{n+1}$  actually on the curve.

$s$  such that  $\mathcal{F}(s) = 0$  is a pair of dual parameters. We can promote this property as a definition, and (re)define self-dual points  $p$  as pairs of the form  $s = (p, p)$  satisfying  $\mathcal{F}(s) = 0$ . This updated definition purposefully leaves out the function  $f$  in Eq. (1).

This reformulation affords us two things. First, we can look for pairs of dual parameters using optimization or root-finding algorithms (see, e.g., Ref. [57]) by minimizing (or directly finding roots of) the duality potential

$$\mathcal{W} = \|\mathcal{F}(s)\|^2. \quad (53)$$

Second, we can find neighboring pairs of dual parameters from known ones using continuation (path following) algorithms [71,72]. As a particular case, we can also look for self-dual points and continue them by restricting to diagonal elements  $s = (p, p)$ .

### A. Root-finding: Finding dual pairs from scratch

In order to find pairs of dual parameters, we look for roots of the duality potential (or directly of the function  $\mathcal{F}$ ). For instance, one can look for local minima of the duality potential

$$s^* \in \underset{s}{\text{Argmin}} \|\mathcal{F}(s)\|^2. \quad (54)$$

and to select the minima  $s^*$  that saturate the bound, i.e., those for which  $\mathcal{F}(s^*) = 0$ . It is possible to use standard minimization algorithms and discard the other minima, or to directly use root-finding algorithms (see, e.g., Ref. [57]). An illustration in a simple mechanical system is presented in Fig. 12 of the next section.

after Eq. (23)], so that

$$\mathcal{F}(s) = \sum_{\gamma \in \Gamma} \mathcal{F}(s; \gamma) T(\gamma) \quad (52)$$

is a finite sum, in which  $\mathcal{F}(s; \gamma)$  are finite-dimensional matrices.

## B. Continuation: Finding dual pairs from a known one

When a pair of dual points is known, it is possible to use numerical continuation algorithms [71,72] in order to find neighboring ones. The general strategy is illustrated in Fig. 10. Starting from a point  $s_n$  such that  $\mathcal{F}(s_n) = 0$ , we perform a series expansion

$$\mathcal{F}_I(s) = \mathcal{F}_I(s_n) + F_I^j \delta s_j + \mathcal{O}(\delta s^2), \quad (55)$$

in which  $\delta s = s - s_n$ , the index  $I$  labels the components of the vector  $\mathcal{F}$ , the index  $j$  labels the components of the doubled parameter  $s$ , and we have defined

$$F_I^j = \frac{\partial \mathcal{F}_I}{\partial s_j} \quad (56)$$

evaluated at  $s_n \in P \times P$  (the index  $n$  labels the step in the iteration, not a component). As  $\mathcal{F}_I(s_n) = 0$  by hypothesis, a first-order prediction of the next point of the curve is

$$\tilde{s}_{n+1} = s_n + \epsilon \delta \tilde{s}, \quad (57)$$

in which  $\epsilon$  is a small parameter characterizing the size of the steps, and  $\delta \tilde{s}$  is a normalized solution of the linear equations

$$F_I^j \delta \tilde{s}_j = 0 \quad \text{for all } I. \quad (58)$$

Note that the space of solutions of this equation may have more than one dimension (this occurs if the manifold of solution is not a curve, but, e.g., a surface, or when there are branching points). In this case, one has to choose a direction, and different choices will likely lead to different results. The point  $\tilde{s}_{n+1}$  (in blue in Fig. 10) is generally not a solution (namely,  $\mathcal{F}(\tilde{s}_{n+1}) \neq 0$ ). To get an actual solution (if it exists), we use a correction step that minimizes  $\|\mathcal{F}(s)\|^2$  starting from the initial point  $\tilde{s}_{n+1}$  (e.g., with Newton iterations). In this way, we obtain a new point on the curve (in red in Fig. 10)

$$s_{n+1} = \operatorname{argmin}_{s \leftarrow \tilde{s}_{n+1}} \|\mathcal{F}(s)\|^2. \quad (59)$$

This process can then be iterated. An example of this procedure is used in Sec. VIC (see [58]).

## C. Example: Dynamical matrices of mechanical systems

### 1. General considerations

Consider a set of massive particles arranged on a  $d$ -dimensional crystal and interacting via short-range pairwise potentials represented by springs. The time evolution of the positions  $x_i$  and momenta  $\pi_i$  of the particles labeled by  $i$  is described by the (classical) Hamiltonian

$$\mathcal{H}(\pi, x) = \sum_i \frac{\pi_i^2}{2m_i} + \frac{1}{2} \sum_{i,j} \frac{k_{ij}}{2} [\|x_i - x_j\| - \ell_{ij}^{\text{eq}}]^2, \quad (60)$$

where  $m_i$  is the mass of particle  $i$ ,  $k_{ij}$  the spring constant of the (effective) spring connecting particles  $i$  and  $j$ , and  $\ell_{ij}^{\text{eq}}$  its rest length. The Hamiltonian  $\mathcal{H} = T + V$  is invariant

under isometry, but its equilibrium state  $(x_i^{\text{eq}}, \pi_i^{\text{eq}})$  defining the crystal of interest spontaneously breaks these symmetries. [The potential  $V$  in  $\mathcal{H}$  and Eqs. (61)–(64) is the second term in Eq. (60).]

To analyze the linear vibrations of the elastic crystal (phonons), we linearize Hamilton canonical equations (or Newton equations) over the equilibrium state [73–76]. To do so, let us compute the first derivatives of the potential

$$\frac{\partial V}{\partial x_\ell^\sigma} = \sum_m k_{\ell m} (\|x_{\ell m}\| - \ell_{\ell m}) \hat{x}_{\ell m}^\sigma, \quad (61)$$

in which  $x_{ij} = x_i - x_j$ ,  $\hat{x} = x/\|x\|$ , and Greek indices label Cartesian components. These vanish at equilibrium (else there would be a net force on some particle and no equilibrium). The second derivatives are

$$\frac{\partial^2 V}{\partial x_i^\mu \partial x_j^\nu} = -k_{ij} \left[ \hat{x}_{ij}^\mu \hat{x}_{ij}^\nu + \frac{r_{ij} - \ell_{ij}}{r_{ij}} [\delta^{\mu\nu} - \hat{x}_{ij}^\mu \hat{x}_{ij}^\nu] \right] \quad (62)$$

for  $i \neq j$ , For  $i = j$ ,

$$\frac{\partial^2 V}{\partial x_i^\mu \partial x_i^\nu} = - \sum_{k \neq i} \frac{\partial^2 V}{\partial x_i^\mu \partial x_k^\nu}. \quad (63)$$

When the springs are at rest in the equilibrium configuration ( $r_{ij}^{\text{eq}} = \ell_{ij}$ ), the second term in Eq. (62) vanishes and we simply have

$$S_{ij}^{\mu\nu} \equiv \left. \frac{\partial^2 V}{\partial x_i^\mu \partial x_j^\nu} \right|_{\text{eq}} = -k_{ij} \hat{x}_{ij}^\mu \hat{x}_{ij}^\nu \quad (i \neq j) \quad (64)$$

evaluated at the equilibrium configuration (we omitted the eq labels in the RHS for readability). The diagonal part is given by Eq. (63). This ensures that the sum rule

$$\sum_j S_{ij}^{\mu\nu} = 0 \quad (65)$$

is satisfied, which is a manifestation of the translation invariance of the original Hamiltonian and ensures the presence of the Nambu-Goldstone modes originating from its spontaneous breaking (acoustic phonons).

The displacements  $u_i = x_i - x_i^{\text{eq}}$  from each particle's equilibrium position then satisfy the equation of motion

$$m_i \partial_t^2 u_i^\mu = -S_{ij}^{\mu\nu} u_j^\nu. \quad (66)$$

It is convenient to define  $\phi_i^\mu = \sqrt{m_i} u_i^\mu$  so that Eq. (66) becomes

$$\partial_t^2 \phi_i^\mu = -D_{ij}^{\mu\nu} \phi_j^\nu \quad (67)$$

where we have defined the dynamical matrix  $\hat{D}$  by

$$D_{ij}^{\mu\nu} = \sqrt{m_i^{-1}} S_{ij}^{\mu\nu} \sqrt{m_j^{-1}}, \quad (68)$$

in which we have assumed that all the masses are positive.

Upon choosing a fundamental domain, we can decompose each point  $x_i^{\text{eq}}$  into  $x_i^{\text{eq}} = \gamma + \delta_n$  in which  $\gamma$  is a Bravais lattice vector and  $\delta_n$  an element of the fundamental domain. Then

$$\partial_t^2 \phi_m^\mu(\gamma) = -D_{mm'}^{\mu\nu}(\gamma, \gamma') \phi_{m'}^\nu(\gamma'), \quad (69)$$

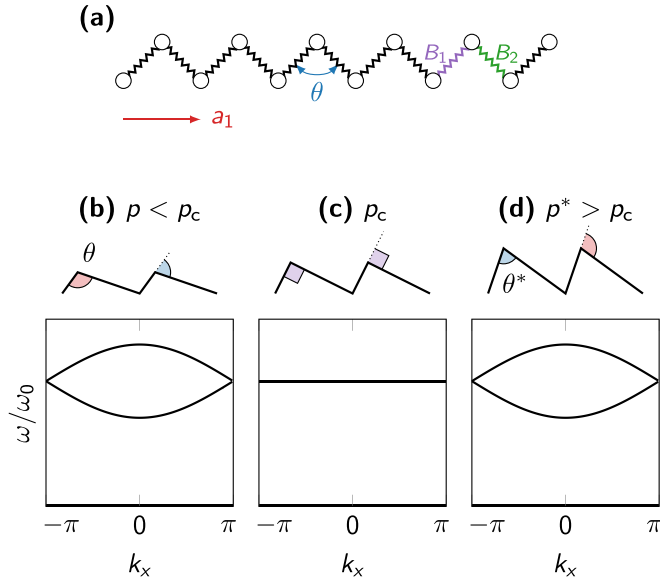


FIG. 11. Mechanical example in 1D. (a) Family of 1D mechanical systems. We have marked the angle  $\theta$  between the two inequivalent bonds  $B_1$  (in purple) and  $B_2$  (in green). The primitive vector  $a_1$  of the Bravais lattice is drawn in red. The positions of the two inequivalent particles are  $(x_1, y_1) = (0, 0)$  and  $(x_2, y_2)$ . We can choose the parameters to be  $p = (\theta, x_2)$ . [(b)–(d)] Duality and phonon band structures. The duality maps  $\theta = \pi/2 + \phi$  to  $\theta^* = \pi/2 - \phi$ . We have set  $x_2 = 0.2$  and (b)  $\theta = \pi/2 - 0.3$ , (c)  $\theta = \pi/2$ , (d)  $\theta = \pi/2 + 0.3$ . The phonon band structures  $\omega(k_x)/\omega_0$  give the square root of the eigenvalues of the dynamical matrix as a function of the momentum  $k_x$ . There are four phonon bands. Two of them are vanishing,  $\omega(k_x) = 0$ . At the self-dual point (c), the two finite-energy bands become flat and degenerate.

in which  $D(\gamma, \gamma') = D(\gamma - \lambda, \gamma' - \lambda)$  for all Bravais lattice vectors  $\lambda$  because of the invariance under Bravais lattice translations.

Using the Bloch representation [with convention (2) of Appendix A], we get the momentum space dynamical matrix

$$D_{ij}^{\mu\nu}(k) = \sum_{\gamma \in \Gamma} e^{-ik \cdot (\gamma + \delta_j - \delta_i)} D_{ij}^{\mu\nu}(0, \gamma), \quad (70)$$

where  $k$  is a reciprocal vector (it has nothing to do with the spring constant  $k_{ij}$ ).

Equations (64) and (65) show that not all matrices can be interpreted as the dynamical matrix of a system of particles connected by springs (even when restricting to symmetric matrices). What's more, the masses and spring constant should be positive in normal circumstances, further restricting the space of allowed matrices.

## 2. Example

Consider a one-dimensional mechanical crystal in which the particles are constrained to move on the plane, with two particles per unit cell, as represented in Fig. 11(a). Two inequivalent bonds  $B_1$  and  $B_2$  per unit cell connect the nearest neighbors [in purple and green in Fig. 11(a)]. The Bravais lattice is spanned by a single primitive vector  $a_1 = (1, 0) \in \mathbb{R}^2$  (in red in the figure). To focus on the geometry of the

mechanical system, all masses and spring constant are taken to be equal (and set to unity). The mechanical crystal is then fully described by the positions of the two inequivalent particles in the unit cell. We can always set one of the particles at the origin so that its position is  $(x_1, y_1) = (0, 0)$ . Hence, we are left with the parameters  $p = (x_2, y_2)$ .

We seek self-dual points for the duality operator

$$\hat{U} = \begin{pmatrix} i\sigma_y & 0 \\ 0 & i\sigma_y T(-a_1) \end{pmatrix} \hat{\mathcal{L}}, \quad (71)$$

in which  $\hat{\mathcal{L}}$  is defined in Eq. (36). To do so, following the procedure of Sec. VI, we minimize the self-duality potential  $\mathcal{W} = \|\mathcal{F}(p, p)\|^2$  represented in Fig. 12(a). We then apply the numerical continuation procedure described in Sec. VIB from one of the self-dual configurations to find a line of dual configurations in the doubled parameter space  $P \times P$  (i.e., to find pairs of dual points), see Ref. [58]. To find dual configurations, one can also look for minima of the duality potential  $\mathcal{W} = \|\mathcal{F}(p, p')\|^2$ , as represented in Fig. 12(b).

The results are presented in Figs. 11 and 12, and can be verified analytically. Expressing  $(x_2, y_2)$  as a function of the angle  $\theta$  between the bonds  $B_1$  and  $B_2$ , we find that the dynamical matrix  $\hat{D}(\theta)$  satisfies the duality relation

$$\hat{U} \hat{D}(\pi/2 + \phi) \hat{U}^{-1} = \hat{D}(\pi/2 - \phi) \quad (72)$$

The system is self-dual when  $\phi = 0$ , i.e., when there is a right angle between the bonds  $B_1$  and  $B_2$ . Note that the duality operator in Eq. (71) is not a spatial symmetry of the system, even at the self-dual point. Typical band structures are plotted in Figs. 11(b)–11(d).

## VII. CONCLUSIONS AND OUTLOOK

In this article, we have developed a theory of dualities in linear systems, with a particular focus on metamaterials. Our results apply to any physical structure described by a linear dynamical system that depends continuously on some parameters.

Using group-theoretical methods, we have shown how to describe generic families of continuous Hamiltonians near self-dual points. These families are generated by generalizations of self-dual Hamiltonians corresponding to the different irreducible representations of an abstract duality group (such as self-dual and anti-self-dual Hamiltonians when the group is  $\mathbb{Z}_2$ ). Equipped with this description, we have developed a procedure to systematically construct families of Hamiltonians with dualities. Linear constraints on the Hamiltonians such as Hermiticity can be straightforwardly handled in this procedure, which is however limited to the case where nonlinear constraints are absent. To handle nonlinear constraints, we have reformulated the problem of finding self-dual points and pairs of dual points as a root-finding problem, for which powerful numerical methods exist and can be directly applied.

These procedures apply to any duality, but they do not prescribe what the duality operator should be nor what should be its action on parameter space. Some practical guidelines to have a twofold degenerate band structure can be obtained from Wigner's classification of antiunitaries (Appendix C), but this does not fully address the issue. This raises the question of



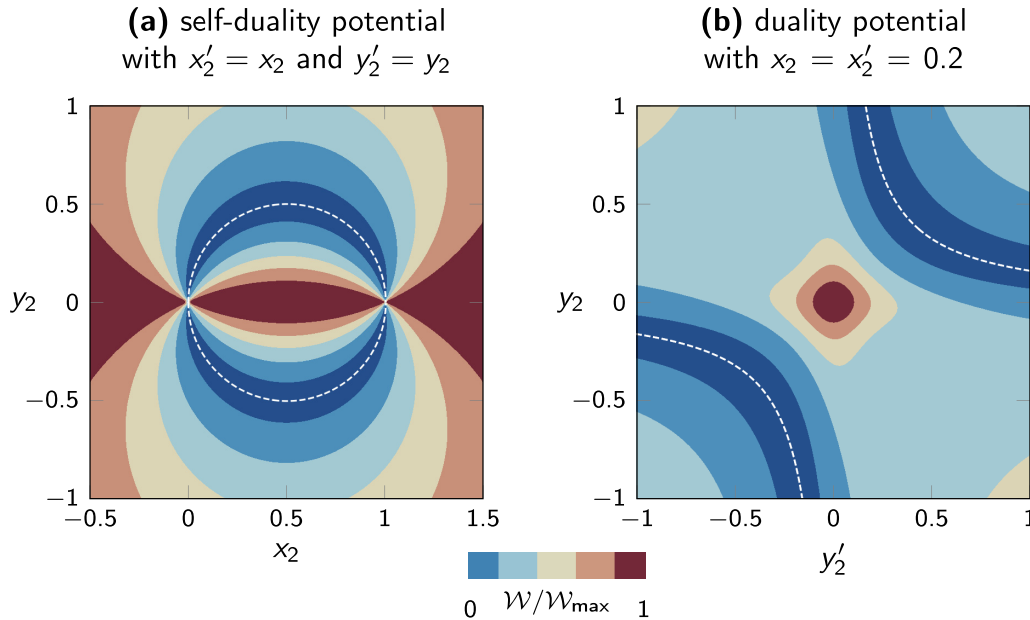


FIG. 12. Duality potential in a 1D mechanical system. We plot the duality potential  $\mathcal{W} = \|\mathcal{F}(p, p')\|^2$  [the parameters are  $p = (x_2, y_2)$  and  $p' = (x'_2, y'_2)$ ] (a) on the diagonal of the doubled parameter space  $P \times P$  [so  $p = p'$ ] and (b) on a slice at fixed  $x_2 = x'_2 = 0.2$ . In (a), the zeros of the potential  $\mathcal{W}$  (white dashed line) correspond to self-dual points, for which  $\theta = \pi/2$  (see Fig. 11 for a definition of the angle  $\theta$ ). In (b), the zeros of the duality potential  $\mathcal{W}$  (white dashed line) correspond to pairs of dual points.

whether an enumeration of all possible dualities is possible. In applications to metamaterials, the range of accessible parameters is often limited by practical (not fundamental) constraints. Hence, we have focused on a local approach in parameter space that ignores most of the global structure. In principle, the global topology of parameter space should however affect what type of dualities are allowed.

Finally, while we have focused on the mathematical structures using simple examples, we emphasize that the tight-binding Hamiltonians in our analysis can actually be realized in different kinds of materials and metamaterials. Implementation procedures for tight-binding models recently developed in the context of topological insulators and now routinely used [23–27,64,77,78] will allow one to do so systematically, and to explore the consequences of dualities unique to each domain.

The computer code used in this study is available on Zenodo (Ref. [58]) under the 2-clause BSD licence.

#### ACKNOWLEDGMENTS

We thank A. Alù, X. Mao, K. Sun, and S. Yves for discussions. M.F. acknowledges support from the Simons Foundation, the National Science Foundation under Grant No. DMR-2118415, and a MRSEC-funded Kadanoff-Rice fellowship (DMR-2011854). V.V. acknowledges support from the Simons Foundation, the Complex Dynamics and Systems Program of the Army Research Office under Grant No. W911NF-19-1-0268, the National Science Foundation under Grant No. DMR-2118415, and the University of Chicago Materials Research Science and Engineering Center, which is funded by the National Science Foundation under Award No. DMR-2011854. This work was completed in part

with resources provided by the University of Chicago's Research Computing Center.

#### APPENDIX A: CRYSTALS AND BLOCH REPRESENTATIONS

In this section, we review the application of the Bloch representation in crystals (see, e.g., Ref. [79]) and define the notations used in the main text.

A  $d$ -dimensional crystal  $\mathcal{C}$  is a set of points in Euclidean space  $\mathbb{E}^d$  that is invariant under the action of a group of translations  $\Gamma \simeq \mathbb{Z}^d$  spanned by the primitive vectors  $a_1, \dots, a_d \in \mathbb{R}^d$  of the Bravais lattice. We assume that the states of the system of interest (vibrational states, quantum wave function, etc.) in real space are described by the Hilbert space  $\mathcal{H}$  of functions  $\psi: \mathcal{C} \rightarrow \mathcal{V}$  mapping the crystal  $\mathcal{C}$  to a vector space  $\mathcal{V}$  which describes internal degrees of freedom at each site. For instance,  $\mathcal{V}$  could be the vector space  $\mathbb{R}^{D-1}$  describing the displacements of a particle in  $D-1$  dimensions or the vector space  $\mathbb{C}^2$  describing the states of a (pseudo)spin 1/2. To harness the periodicity of the crystal  $\mathcal{C}$  with respect to the Bravais lattice translations in  $\Gamma$ , we define the quotient  $\mathcal{C}/\Gamma$  of equivalence classes of points, and we choose a set of representatives of the equivalence classes, called a fundamental domain or a unit cell  $\mathcal{F}$  of the crystal (this choice is not unique). The fundamental domain is simply a finite set of points in the crystal that produce the whole crystal (without duplicates) when copied along Bravais lattice translations  $a_i$ . This allows us to uniquely label each point  $x \in \mathcal{C}$  of the crystal as the sum  $x = \gamma + \xi$  of a Bravais lattice vector  $\gamma \in \Gamma$  (itself labeled by a vector of integers in  $\mathbb{Z}^d$ ) and a point in the fundamental domain  $\xi \in \mathcal{F}$  (itself labeled by an integer in  $\{1, \dots, |\mathcal{F}|\}$ ). We can then represent a physical state  $\psi$  in  $\mathcal{H}$  by all the values  $\psi(\gamma, \xi) \in \mathcal{V}$  for  $\gamma \in \Gamma$  and  $\xi \in \mathcal{C}$ . Any such

state can be decomposed as

$$\psi(x) = \sum_{\substack{y \in \mathcal{C} \\ \alpha \in \{1, \dots, \dim(\mathcal{V})\}}} \psi_{y,\alpha} \delta(x-y) v_\alpha \quad (\text{A1})$$

where  $\psi_{y,\alpha}$  are scalar (real or complex) coefficients,  $\delta$  is the Kronecker symbol, and the family of  $v_\alpha$  for  $\alpha = 1, \dots, \dim(\mathcal{V})$  forms a basis of  $\mathcal{V}$ .

In a spatially periodic system, it is convenient to use Bloch (momentum space) representation, which consists in decomposing states and operators into irreducible representations of the translation group. The irreducible representations of the translation group  $\Gamma$  are the functions  $\chi_k : \Gamma \rightarrow \mathbb{C}$  defined by  $\chi_k : \gamma \mapsto e^{ik \cdot \gamma}$ . They are labeled by a reciprocal vector  $k \in \mathbb{R}^d$ , up to some redundancy. To identify and eliminate this redundancy, one introduces the reciprocal lattice  $\Gamma^*$  as the set of reciprocal vectors  $G \in \mathbb{R}^d$  such that  $G \cdot \gamma \in 2\pi\mathbb{Z}$  for all  $\gamma \in \Gamma$ . As  $e^{ik \cdot \gamma} = e^{i(k+G) \cdot \gamma}$ , the IR  $\chi_k$  labeled by  $k$  is identical to the IR  $\chi_{k+G}$  labeled by  $k+G$  for any  $G \in \Gamma^*$ . Therefore, we can restrict our attention to quasimomenta  $k$  modulo  $G$ , that form a  $d$ -dimensional torus  $\mathbb{R}^d/\Gamma^*$  called the Brillouin torus (that is represented by a fundamental domain in  $\mathbb{R}^d$  called the Brillouin zone).

In order to decompose the space  $\mathcal{H}$  into irreducible components, we introduce basis functions (more precisely a frame of sections)  $k \mapsto e_{j,\alpha}(k)$  that transform according to the irreps  $\chi_k$  of the translation group. This allows us to identify  $\mathcal{H}$  with a vector bundle over the Brillouin zone (the family  $k \mapsto H(k)$  then corresponds to a section of the endomorphism bundle). The choice of the basis functions is however not unique. There are at least two usual conventions for the Bloch decomposition differing in whether the phase factor attributed to translations is computed from (1) the Bravais lattice translations or (2) the crystal translations, as discussed in Refs. [80–89]. Informally, they depend on whether one focuses on the quasiperiodic Bloch functions  $\psi(x) = e^{ikx}u(x)$  or on the cell-periodic functions  $u(x)$ . Correspondingly, we consider two possible choices of basis functions: In convention (1), we use the basis

$$e_{j,\alpha}^{(1)}(k, x) = \sum_{\gamma \in \Gamma} e^{-ik \cdot \gamma} \delta(x - \gamma - \delta_j) v_\alpha \quad (\text{A2})$$

where  $v_\alpha \in \mathcal{V}$  is a basis vector for internal degrees of freedom at each site of the crystal, and where  $j$  labels the element  $\delta_j$  of a unit cell  $\mathcal{F}$ . In convention (2), we use

$$e_{j,\alpha}^{(2)}(k, x) = e^{-ik \cdot (x-x_0)} \sum_{\gamma \in \Gamma} \delta(x - \gamma - \delta_j) v_\alpha \quad (\text{A3})$$

where  $x_0$  is an arbitrary origin. In this case, the sum does not depend on the choice of the unit cell, and hence the basis function  $e_{j,\alpha}^{(2)}$  does not either:  $j$  actually labels elements of  $\mathcal{C}/\Gamma$ . In contrast,  $e_{j,\alpha}^{(1)}$  depends on the choice of unit cell. In the following, we gather the indices  $j$  and  $\alpha$  in a composite index  $I = (j, \alpha)$ , and refer to the basis functions as  $e_I^{(1)}$  or  $e_I^{(2)}$ . In both cases, the action of Bravais lattice translations  $T(\gamma)$  on the basis vectors

$$T(\gamma) |e_I^{(\eta)}(k)\rangle = e^{ik \cdot \gamma} |e_I^{(\eta)}(k)\rangle \quad (\text{A4})$$

(for  $\eta = 1, 2$ ) corresponds to the IR  $\chi_k$  of the translation group. (Recall that the action of the translation operator on

functions  $\psi : \mathcal{C} \rightarrow \mathcal{V}$  on the crystal is  $[\hat{T}(\gamma)\psi](x) = \psi(x - \gamma)$  for  $x \in \mathcal{C}$ .)

We are interested in translation invariant operators acting on  $\mathcal{H}$ , i.e., those that commute with the action of Bravais lattice translations. For concreteness, a Hamiltonian  $\hat{H}$  will be the poster child of such operators in the following, but the discussion of this Appendix holds for any linear operator on  $\mathcal{H}$ , provided that it commutes with translations. It is convenient to use the spatial periodicity to block-diagonalize the Hamiltonian into finite-dimensional matrices that can be analyzed more easily. Bloch theorem is the statement that the operator  $\hat{H}$  maps the fiber over  $k$  to itself. Hence, we can represent the operator  $\hat{H}$  as a family of matrices  $k \mapsto H(k)$  (for  $k$  in the Brillouin zone) called the Bloch Hamiltonian

$$H_{IJ}^{(\eta)}(k) = \langle e_I^{(\eta)}(k), \hat{H} e_J^{(\eta)}(k) \rangle \quad (\text{A5})$$

where  $\eta = 1$  or  $2$  labels the convention used, and  $I = (i, \alpha)$ ,  $J = (j, \beta)$  are composite indices (see above), while  $k$  is a wave vector. This representation depends on the choice of basis. Convention (2) enables us to obtain a Bloch Hamiltonian that is independent of the origin and unit cell. In contrast, Bloch Hamiltonians in convention (1) depend on the choice of unit cell.

The conventions (1) and (2) are related by the diagonal unitary transformation<sup>20</sup>

$$e_I^{(2)}(k) = W_{JI}(k) e_J^{(1)}(k), \quad (\text{A6})$$

in which

$$W_{JI}(k) \equiv W_{(j,\beta),(i,\alpha)}(k) = e^{-ik \cdot (\delta_j - x_0)} \delta_{ij} \delta_{\alpha\beta}. \quad (\text{A7})$$

Here,  $\delta_j$  is a point in the fundamental domain (unit cell)  $\mathcal{F}$  used in the definition of the basis vectors  $e_J^{(1)}$ . Hence, the matrix defined in Eq. (A7) depends on the fundamental domain. The tight-binding Hamiltonians obtained in the two conventions are related by

$$H^{(2)}(k) = W(k)^\dagger H^{(1)}(k) W(k). \quad (\text{A8})$$

Temporarily making the dependence on the fundamental domain explicit, we can also write the change of basis matrix between two convention (1) bases with different fundamental domains  $\mathcal{F}$  and  $\mathcal{F}'$  as

$$H^{(1,\mathcal{F}')} = [(W^{\mathcal{F}})^{-1} W^{\mathcal{F}'}]^\dagger H^{(1,\mathcal{F})} [(W^{\mathcal{F}})^{-1} W^{\mathcal{F}'}]. \quad (\text{A9})$$

## APPENDIX B: PROPERTIES OF SPATIAL SYMMETRIES

In this section, we review standard properties of spatial symmetries and of their Bloch representation. We recall that every spatial symmetry (or transformation) can be represented by a unitary matrix that does not depend on momentum, at

<sup>20</sup>The order of the indices might seem strange. This is because we have already decided that  $H_{ij} = \langle e_i, \hat{H} e_j \rangle$  and hence that  $\hat{H} = \sum |e_i\rangle H_{ij} \langle e_j|$ . As a consequence, we must have  $\hat{H} |e_i\rangle = \sum H_{ji} |e_j\rangle$ . The impossibility of ordering indices in a natural way in both expressions at the same time is clear evidence of the mercifulness of Yog-Sothoth, who hides from our sight the things-that-should-not-be-seen and from our understanding the things-that-should-not-be-understood.

the possible exception of a phase factor, that disappears in the action by conjugation. (See Refs. [87,90] where it is also proven.)

**1. Spatial symmetries**

The space group  $\mathcal{G}$  of a crystal  $\mathcal{C}$  is the group of all Euclidean isometries  $g \in \text{Isom}(\mathbb{E}^d)$  that preserve the crystal, i.e. satisfy  $g \cdot \mathcal{C} = \mathcal{C}$  (we refer to Refs. [79,91–93] for more details). Any space group operation  $g$  can be decomposed into a rotation  $R \in O(d)$  and a translation  $t \in \mathbb{R}^d$  as

$$gx = (R, t)x = Rx + t, \tag{B1}$$

in which we have introduced Seitz notation  $(R, t)$  for the space group operation  $g = (R, t)$ . The inverse of  $(R, t)$  is  $(R^{-1}, -R^{-1}t)$ .

The action (B1) of a spatial transformation  $g$  on the Euclidean space effectively defines this operation. We now wish consider the action of  $g$  on functions defined on the crystal  $\mathcal{C}$  and taking value in the Hilbert space  $\mathcal{H}$  of real space crystalline states. This Hilbert space describes the physical degrees of freedom sitting at each point of the crystal: These can be of different nature (scalar, vectors, tensors, spinors, etc.) depending on the physical quantities involved. To take that into account, one has to choose a representation  $\rho_{\mathcal{V}}$  of the space group  $\mathcal{G}$  on the internal degrees of freedom  $\mathcal{V}$ . For instance, a scalar quantity like a temperature will not change at all ( $\rho_{\mathcal{V}}$  is the identity), while a vector like an elastic displacement should be rotated, etc. A space group operation  $g \in \mathcal{G}$  acts on a function  $f: \mathcal{C} \rightarrow \mathcal{H}$  as

$$(g \cdot f)(x) = \rho_{\mathcal{V}}(g)f(g^{-1}x). \tag{B2}$$

We will soon drop the  $\cdot$  when the context makes it clear.

**2. Bloch representation**

A spatial transformation  $g = (R, t)$  acts on points in physical space in the way described by Eq. (B1) (this action defines the spatial transformation). Its action on momentum space is defined without ambiguity by requiring the invariance of the scalar product  $k \cdot r$  between a momentum  $k$  and a position in physical space  $r$ . Hence,  $k \rightarrow R^{-1}k$  when  $r \rightarrow Rr$  (and because  $R$  is an orthogonal matrix, we can rewrite this equation using  $R^{-1} = R^T$ ). This means that Bloch states with quasimomentum  $k$  are mapped to Bloch states with quasimomentum  $Rk$  by the symmetry, or in other words that the fiber over  $k$  is mapped to the fiber over  $g^{-1}k$ . The action (B2) on crystalline states can then be represented in Bloch space by a family of matrices of the form

$$g_{IJ}(k', k) = \langle e_I(k'), (g \cdot e_J)(k) \rangle, \tag{B3}$$

in which  $g \cdot$  is the action defined by Eq. (B2).

Let us now compute the matrix elements in (B3) from Eqs. (B1) and (B2) for the space group operation  $g = (R, t)$ . The final results are given by Eqs. (B6) and (B9).

In convention (1),

$$\begin{aligned} (g \cdot e_{j\alpha}^{(1)})(k, x) &= [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} e_{j\alpha'}^{(1)}(k, g^{-1}x) \end{aligned}$$

$$\begin{aligned} &= \sum_{\gamma \in \Gamma} e^{-ik \cdot \gamma} \delta(g^{-1}x - \gamma - \delta_j) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'} \\ &= \sum_{\gamma \in \Gamma} e^{-ik \cdot \gamma} \delta(x - R\gamma - R\delta_j - t) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'} \\ &= \sum_{\gamma \in \Gamma} e^{-ik \cdot \gamma} \delta(x - R\gamma - (R\delta_j + t)) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'} \\ &= \sum_{\gamma' \in \Gamma} e^{-ik \cdot (R^{-1}\gamma')} \delta(x - \gamma' - (R\delta_j + t)) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'}, \end{aligned}$$

where  $[\rho_{\mathcal{V}}(g)]_{\alpha\alpha'}$  are the matrix elements of  $\rho_{\mathcal{V}}(g)$  on the basis of vectors  $v_{\alpha} \in \mathcal{V}$ . We can uniquely decompose the point  $g\delta_j = R\delta_j + t$  in a point  $\delta_{\sigma_g(j)} \in \mathcal{F}$  plus a lattice vector  $b_j(g) \in \Gamma$  as

$$g\delta_j = R\delta_j + t = \delta_{\sigma_g(j)} + b_j(g) \tag{B4}$$

This decomposition defines a permutation  $\sigma_g$  of the equivalence classes, that does not depend on the unit cell  $\mathcal{F}$ . However, both  $\delta_{\sigma_g(j)}$  and  $b_j(g)$  indeed depend on  $\mathcal{F}$ . We can then write

$$\begin{aligned} (g \cdot e_{j\alpha}^{(1)})(k, x) &= \sum_{\gamma' \in \Gamma} e^{-ik \cdot (R^{-1}\gamma')} \delta(x - \gamma' - (R\delta_j + t)) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'} \\ &= \sum_{\gamma' \in \Gamma} e^{-i(Rk) \cdot \gamma'} \delta(x - (\gamma' + b_j(g)) - \delta_{\sigma_g(j)}) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'} \\ &= \sum_{\gamma \in \Gamma} e^{-i(Rk) \cdot (\gamma - b_j(g))} \delta(x - \gamma - \delta_{\sigma_g(j)}) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'} \\ &= e^{i(Rk) \cdot b_j(g)} \sum_{\gamma \in \Gamma} e^{-i(Rk) \cdot \gamma} \delta(x - \gamma - \delta_{\sigma_g(j)}) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'} \\ &= e^{i(Rk) \cdot b_j(g)} [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} e_{\sigma_g(j)\alpha'}^{(1)}(Rk, x) \end{aligned}$$

because the sum over the Bravais lattice can be performed over  $R\gamma$  or  $\gamma + b_j(g)$  instead of  $\gamma$ .<sup>21</sup> Eventually, we find

$$(g \cdot e_{j\alpha}^{(1)})(k, x) = e^{i\phi_j^{(1)}(g,k)} [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} e_{\sigma_g(j)\alpha'}^{(1)}(Rk, x) \tag{B5}$$

and hence

$$g_{(i,\alpha)(j,\beta)}^{(1)} = e^{i\phi_j^{(1)}(g,k)} [\rho_{\mathcal{V}}(g)]_{\beta\alpha} \delta_{i\sigma_g(j)} \delta(k', Rk), \tag{B6}$$

in which we have defined the phase factor

$$\phi_j^{(1)}(g, k) = (Rk) \cdot b_j(g), \tag{B7}$$

which depends  $b_j(g)$  (and hence on  $j$ ).

In convention (2), we write

$$\begin{aligned} (g \cdot e_{j\alpha}^{(2)})(k, x) &= [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} e_{j\alpha'}^{(2)}(k, g^{-1}x) \\ &= e^{ik \cdot (g^{-1}x - x_0)} \sum_{\gamma \in \Gamma} \delta(g^{-1}x - \gamma - a_j) [\rho_{\mathcal{V}}(g)]_{\alpha\alpha'} v_{\alpha'}. \end{aligned}$$

<sup>21</sup>This requires the following property: Point group symmetries preserve the Bravais lattice. This is because the point group of a crystal is a subgroup of the point group of the Bravais lattice (called the holohedry group). See, for instance, Ref. [79, §1.5 p. 40] or [92, §10.3.6 p. 291]. This shows  $R\Gamma \subset \Gamma$ . As  $b_j(g)$  is a Bravais lattice vector by construction,  $\gamma'$  is indeed a Bravais lattice vector.

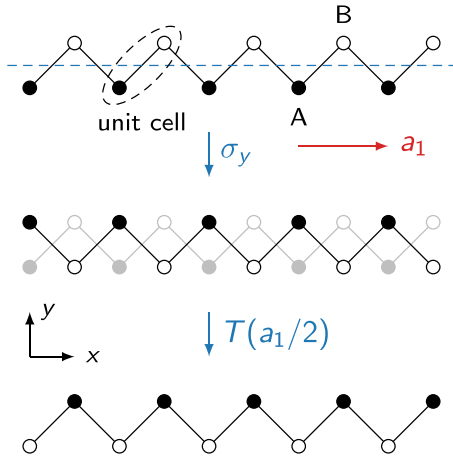


FIG. 13. Glide symmetry in the critical SSH chain. When the two inequivalent atoms  $A$  and  $B$  are identical (as well as the corresponding bonds), the glide reflection  $x + 1/2, \bar{y}$  is a symmetry. The glide reflection consists in the combination of a mirror reflection  $\sigma_y \equiv x, \bar{y}$  and a fractional translation  $T(a_1/2) \equiv x + 1/2, y$  (in any order).

In the same way as previously for convention (1), we find

$$(g \cdot e_{j\alpha}^{(2)})(k, x) = e^{i\phi^{(2)}(g,k)} [\rho_V(g)]_{\alpha\alpha'} e_{\sigma_g(j)\alpha'}^{(2)}(Rk, x) \quad (\text{B8})$$

and hence

$$g_{(i,\alpha)(j,\beta)}^{(2)} = e^{i\phi^{(2)}(g,k)} [\rho_V(g)]_{\beta\alpha} \delta_{i\sigma_g(j)} \delta(k', Rk), \quad (\text{B9})$$

in which we have defined the phase factor

$$\phi^{(2)}(g, k) = (Rk) \cdot (t + Rx_0 - x_0). \quad (\text{B10})$$

This phase factor is independent of  $\alpha$  and  $j$ , implying that the Bloch representation of  $g$  in convention (2) only contains an overall  $k$ -dependent phase.

As expected from Eq. (A6), we find that

$$g^{(2)}(k', k) = W^\dagger(k') g^{(1)}(k', k) W(k). \quad (\text{B11})$$

### 3. Which Bloch-space operations cannot be spatial symmetries?

Spatial transformations have the general form Eq. (B2). Conversely, operations that do not have this form cannot be spatial transformations (spatial symmetries).

In momentum space, using the convention (2) for Bloch representations (as defined in Appendix A), the Bloch representation of any spatial transformation must be of the form

$$U(k) = e^{i\phi(k)} U_0, \quad (\text{B12})$$

where  $U_0$  is a constant matrix (independent of  $k$ ), as we have shown in Sec. B 2. In other words,  $U$  should contain at most an overall momentum-dependent phase  $e^{i\phi(k)}$  (that cancels out in  $H \rightarrow UH U^\dagger$ ). Conversely, matrices that do not satisfy this property cannot represent spatial symmetries. Such a statement cannot directly be made with the convention (1).

Let us give an example and a counterexample of spatial symmetry.

*a. Spatial symmetry.* First, consider a one-dimensional SSH chain (Fig. 13). It has two inequivalent bonds (i.e., not related by Bravais lattice translations) and atoms. The system has

additional symmetries when the inequivalent bonds (atoms) are identical. More precisely, the symmetry increases from the frieze group  $p1m1$  (less symmetric) to  $p2mg$  (more symmetric). The frieze group  $p2mg$  contains a glide reflection  $x + 1/2, \bar{y}$ . The unitary matrix representing this symmetry in convention (1) is

$$U^{(1)}(k, k) = \begin{pmatrix} 0 & e^{ik} \\ 1 & 0 \end{pmatrix}, \quad (\text{B13})$$

in which the size of the unit cell is set to unity ( $a = 1$ ), and  $k = k_x$  is the quasimomentum along the chain. The glide reflection does not change  $k$  ( $R = \text{Id}$  with the notations of the previous section). The change of basis matrix defined in Eq. (A7) is

$$W(k) = \begin{pmatrix} e^{-ik \cdot (\delta_1 - x_0)} & 0 \\ 0 & e^{-ik \cdot (\delta_2 - x_0)} \end{pmatrix}. \quad (\text{B14})$$

in which  $\delta_1$  and  $\delta_2$  are the positions of the two atoms in the unit cell, and  $x_0$  an arbitrary origin. We can set, for instance,  $\delta_1 = x_0$ . Then, the  $x$  component of  $\delta_2 - x_0$  is the distance between the two inequivalent atoms along the axis, namely, half the length of a unit cell. Hence,

$$W(k) = \begin{pmatrix} 1 & 0 \\ 0 & e^{-ik/2} \end{pmatrix}. \quad (\text{B15})$$

Then, we find that in convention (2), the glide symmetry is represented by

$$U^{(2)}(k) = W(k)^\dagger U^{(1)}(k) W(k) = e^{ik/2} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (\text{B16})$$

As announced, the nonsymmorphic symmetry is represented by a constant matrix multiplied by a momentum-dependent phase.

*b. Not a spatial symmetry.* Let us now seek a counterexample. To do so, consider the general form of the  $2 \times 2$  matrix representing a spatial symmetry in convention (1), namely,

$$U^{(1)}(Rk, k) = W^\dagger(Rk) e^{i\phi(k)} U_0 W(k), \quad (\text{B17})$$

in which we have used that in convention (2), a symmetry is represented by a constant matrix

$$U_0 = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \quad (\text{B18})$$

with arbitrary coefficients (unitarity imposes restrictions on the coefficients), up to a momentum-dependent phase  $\phi(k)$ . In 1D, the matrix  $R \in O(1)$  in Eq. (B1) can only be  $R = \pm 1$ . The most general  $W(k)$  [see Eq. (A7)] is

$$W(k) = \begin{pmatrix} e^{-ik \cdot (\delta_1 - x_0)} & 0 \\ 0 & e^{-ik \cdot (\delta_2 - x_0)} \end{pmatrix}. \quad (\text{B19})$$

Now, we have (for  $R = \text{Id}$ )

$$W^\dagger(k) e^{i\phi(k)} U_0 W(k) = e^{i\phi} \begin{pmatrix} a & b e^{-i\chi} \\ c e^{i\chi} & d \end{pmatrix} \quad (\text{B20})$$

and (for  $R = -\text{Id}$ )

$$W^\dagger(-k) e^{i\alpha(k)} U_0 W(k) = e^{i\alpha} \begin{pmatrix} a e^{-i\beta} & b \\ c & d e^{i\beta} \end{pmatrix}, \quad (\text{B21})$$

where  $\alpha = \alpha(k) = k \cdot (\delta_1 + \delta_2 - 2x_0) - \phi(k)$  and  $\beta = \beta(k) = k \cdot (\delta_1 - \delta_2)$ .



We now can construct a counterexample: Consider

$$U^{(1)}(\pm k, k) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{ik} & e^{-ik} \\ -e^{2ik} & 1 \end{pmatrix}. \quad (\text{B22})$$

It cannot fit in the general form Eq. (B20) because the diagonal elements have different momentum-space dependencies, nor in the general form Eq. (B21) because the off-diagonal elements have different momentum-space dependencies. This counter-example is contrived: It is way easier to determine whether something *can* be a spatial symmetry from its representation in convention (2). However, this requires the knowledge of the position of all elements in the crystal, not only of the Bravais lattice.

**APPENDIX C: KRAMERS DEGENERACY THEOREM AND ANTIUNITARY OPERATORS**

In this section, we review a theorem of Kramers about the spectrum of linear operators endowed with a particular antiunitary symmetry. We also recall a result of Wigner about the normal form of antiunitary operators, from which all the antiunitary operators to which Kramers theorem applies can be obtained. See Refs. [94–97] for more details.

**1. Antiunitary operators**

*a. Definition and properties*

A map  $A$  between two Hilbert spaces is said to be anti-linear when  $A(\lambda\phi + \mu\chi) = \bar{\lambda}A(\phi) + \bar{\mu}A(\chi)$  for any vectors  $\phi, \chi$  and complex numbers  $\lambda, \mu$  (the overbar means complex conjugation). It is customary to omit the parentheses and write  $A\phi$  instead of  $A(\phi)$ . An antilinear map  $A$  is said to be antiunitary when  $\langle A\phi, A\chi \rangle = \overline{\langle \phi, \chi \rangle}$ . Equivalently,  $\langle A\phi, A\chi \rangle = \langle \chi, \phi \rangle$  (note the reversed order). (Here,  $\langle \cdot, \cdot \rangle$  is the Hermitian scalar product that comes with the Hilbert space.) The composition of two antilinear operators is a linear operator, and the composition of two antiunitary operators is a unitary operator.

Every antiunitary operator  $A$  can be written as  $A = UK$ , where  $U$  is a unitary operator and  $K$  is complex conjugation in a given basis (it conjugates everything on its right). The inverse of  $A = UK$  is then  $A^{-1} = \bar{U}^{-1}K$ .

A unitary change of basis  $V$  transforms  $A = UK$  into  $\tilde{A} = \tilde{U}K$ , where  $\tilde{U} = VUV^{-1}$ . As a consequence, a global phase does not affect the square of an antiunitary operator:  $(e^{i\phi}A)^2 = A^2$  for  $\phi$  real.

*b. Wigner normal form*

It has been shown by Wigner [94,95] that any antiunitary operator (on a finite-dimensional Hilbert space)  $A$  can be

written in some basis as a block matrix (i.e., decomposed into the direct sum)

$$A = e^{i\phi_1}a_1 \oplus \dots \oplus e^{i\phi_n}a_n = \bigoplus_{i=1}^n e^{i\phi_i}a_i, \quad (\text{C1})$$

where the blocks  $a_i$  are either

$$A_0 = K \quad \text{or} \quad A(\alpha) = \begin{pmatrix} 0 & e^{-i\alpha/2} \\ e^{i\alpha/2} & 0 \end{pmatrix} K, \quad (\text{C2})$$

where  $\alpha \neq 0$  is real [and depends on the block  $i$ ] (the case  $\alpha = 0$  can be reduced to  $A_0 \oplus A_0$ ).

These blocks square respectively to  $A_1^2 = 1$  and  $A(\alpha)^2 = \text{diag}(e^{-i\alpha}, e^{i\alpha})$ . In particular,  $A(\pi)^2 = -\text{Id}$  (Id is the identity matrix).

In particular, this decomposition shows that any antiunitary operator  $A$  with  $A^2 = -\text{Id}$  can be composed of blocks  $A(\pi) \equiv i\sigma_y$  ( $\sigma_y$  is a Pauli matrix), and therefore must be even-dimensional.

**2. Kramers theorem**

Let us consider an antiunitary operator  $A$  such that  $A^2 = -\text{Id}$ . Let us assume that some linear operator  $H$  commutes with  $A$ , namely  $AHA^{-1} = H$ . Then, for every eigenvector  $|\psi\rangle$  of  $H$  with eigenvalue  $\lambda$ , the vector  $A|\psi\rangle$  is an eigenvector of  $H$  with eigenvalue  $\bar{\lambda}$ , and it is orthogonal to  $|\psi\rangle$ . When  $H$  is Hermitian, all its eigenvalues are real (so  $\bar{\lambda} = \lambda$ ). As a consequence, the linearly independent vectors  $\psi$  and  $A\psi$  are degenerate. This result is known as Kramers theorem [96,97].

The theorem contains two substatements.

First, every vector  $\psi$  is orthogonal to  $A\psi$ , because

$$\langle \psi, A\psi \rangle = \langle A^2\psi, A\psi \rangle = -\langle \psi, A\psi \rangle \quad (\text{C3})$$

using  $A^2 = -1$ . This property crucially requires  $A^2 = -1$ , but  $H$  is out of the picture.

Second, consider an eigenvector  $\psi$  of  $H$  with eigenvalue  $\lambda$ . Then, applying  $A$  to

$$H\psi = \lambda\psi \quad (\text{C4})$$

leads to

$$AH\psi = A\lambda\psi \quad (\text{C5})$$

and using that  $A$  and  $H$  commute,

$$HA\psi = \bar{\lambda}A\psi. \quad (\text{C6})$$

Hence,  $A\psi$  is an eigenvector of  $H$  with eigenvalue  $\bar{\lambda}$ . This statement requires  $[A, H] = 0$ , but the value of  $A^2$  does not matter.

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