Derivation of the Dirac equation from principles of information processing

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Without using the relativity principle, we show how the Dirac equation in three space dimensions emerges from the large-scale dynamics of the minimal nontrivial quantum cellular automaton satisfying unitarity, locality, homogeneity, and discrete isotropy. The Dirac equation is recovered for small wave vector and inertial mass, whereas Lorentz covariance is distorted in the ultrarelativistic limit. The automaton can thus be regarded as a theory unifying scales from Planck to Fermi. A simple asymptotic approach leads to a dispersive Schrödinger equation describing the evolution of narrowband states at all scales.

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I. INTRODUCTION

Since the beginning of the path-integral approach [1], discrete versions of quantum field theories have been extensively studied, giving the Dirac equation in the continuum limit [2,3], and similar models have been developed for simulating Fermi gas on a lattice [4,5]. A special case of discrete theory is the quantum cellular automaton (QCA), the quantum version of the classical cellular automaton of von Neumann [6] (for a review, see Ref. [7]). The two main features of the automaton are (1) the dynamics involve countable systems and (2) the update rule for the state of system is local; namely, in the quantum case it is described by local unitary operators, each one involving few systems. This should be contrasted with other discrete theories—e.g., lattice gauge theories—where the unitary operator is the exponential of an Hamiltonian involving all systems at a time.

QCAs concretize the Feynman and Wheeler paradigm of "physics as information processing" [8–10]. However, so far only classical automata have been contemplated in such view [11,12]. Taking the QCA as the microscopic mechanism for an emergent quantum field has been recently suggested in Refs. [13–15], along with using it as a framework to unify a hypothetical Planck scale with the usual Fermi scale of high-energy physics. The additional bonus of the automaton framework is that it also represents the canonical solution to practically all issues in quantum field theory, such as all divergences and the problem of particle localizability, all due to the continuum, infinite volume, and Hamiltonian description. [16–18]. Moreover, the QCA is the ideal framework for a quantum theory of gravity, being the automaton theory quantum *ab initio* (the QCA is not derivable by quantizing a classical theory), and naturally incorporates the informational foundation for the holographic principle, a relevant feature of string theories [19,20] and the main ingredient of the microscopic theories of gravity of Jacobson [21] and Verlinde [22]. Finally, a theory based on a QCA assumes no background, but only interacting quantum systems, and space time and mechanics are emergent phenomena.

The assumption of Planck-scale discreteness has the consequence of breaking Lorentz covariance along with all continuous symmetries: These are recovered at the Fermi scale in the relativistic limit in the same way as in the doubly special relativity of Amelino-Camelia [23,24] and the deformed Lorentz symmetry of Smolin and Magueijo [25,26]. Such Lorentz deformations have phenomenological consequences, and possible experimental tests have been recently proposed by several authors [27–30]. The deformed Lorentz group of the automaton has been preliminarily analyzed in Ref. [31].

In analogy with classical cellular automata, the QCA consists of cells of quantum systems interacting with a finite number of other cells, but, differently from the classical case, the evolution is reversible. After early stimulating ideas of Feynman [8], the first QCA was introduced in Ref. [32] and only a decade later entered rigorous mathematical literature [33–37]. A QCA, in principle, can evolve a quantum field that can obey any statistics; however, as we see in this paper, in the present spirit of deriving the theory from information-theoretical principles, the QCA is fundamentally Fermionic. In addition, Fermionic QCA can simulate every other QCA respecting the local structure of interactions (see, e.g., [38–40]), whereas the converse is not true.

The evolution defining the QCA is determined by its action on the whole Fock space. However, being linear in the field, as in the present case, the single-particle sector completely specifies the automaton.

In this paper we show how the Dirac equation in three space dimensions can be derived solely from fundamental principles of information processing, without appealing to special relativity. The Dirac equation emerges from the large-scale dynamics of the minimum-dimension QCA, satisfying unitarity, locality, homogeneity, and discrete isotropy of interactions. Precisely, the Dirac equation is recovered for small wave vector and inertial mass. In Sec. II we show the construction of space starting just from interactions between quantum systems by requiring simple informational principles on the update rule representing the evolution of a QCA. The principles allow us to identify the set of systems of the automaton with the Cayley graph of a group. In Sec. III we specialize our construction to the case of automata over Cayley graphs of Abelian groups. In Sec. IV we derive the only four solutions to the unitarity equations for the case of the bcc lattice, corresponding to the unique Cayley graph of $\mathbb{Z}^3$ supporting a QCA satisfying our

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requirements. We call these solutions Weyl automata, because they give Weyl's equation in the relativistic limit. In Sec. V we show the unique possible way to couple Weyl automata locally in order to obtain a new automaton. We call the resulting QCA a Dirac automaton because it gives Dirac's equation in the relativistic limit. The inequivalent Dirac automata are only two. In Sec. VI we show the same result for the case of Cayley graphs of $\mathbb{Z}^2$ and $\mathbb{Z}$, leading to Weyl and Dirac QCAs in two and one space dimensions, respectively. Finally, in Sec. VII we study the relativistic limit of all the above automata, which consists of taking small wave vectors compared to the Planck length, which is the scale of a lattice step. We then show the first-order corrections to the Dirac dynamics in the $d = 3$ case, due to the discreteness of space time at the Planck scale, and provide the range of possible experimental tests of the corrections. In this section we also provide an analytical description of the QCA for the narrowband states of quantum field theory in terms of a dispersive Schrödinger equation holding at all scales.

II. QCAS AND SYMMETRIES

In the present section we introduce the general construction of space starting from QCA representing interactions among identical Fermionic quantum systems. Let the cellular automaton involve a denumerable set G of systems, conveniently described by Fermionic field operators $\psi_{g,l}$ satisfying the usual anticommutation relations,

$$\{\psi_{g,l},\psi_{g',l'}\} = 0, \quad \{\psi_{g,l},\psi^\dagger_{g',l'}\} = \delta_{g,g'}\delta_{l,l'}. \tag{1}$$

In the following, we denote by ψ_g the formal s_g-component column vector,

$$\psi_g = \begin{pmatrix} \psi_{g,1} \\ \psi_{g,2} \\ \vdots \\ \psi_{g,s_g} \end{pmatrix}, \tag{2}$$

where s_g is the number of field components at site g.

We now assume the following requirements for the interactions defining the QCA evolution: (1) linearity, (2) unitarity, (3) locality, (4) homogeneity, and (5) isotropy.

By linearity, we mean that the interaction between systems is described by $s_{g'} \times s_g$ *transition matrices* $A_{gg'}$, which allow us to write the evolution from step t to step $t+1$ as

$$\psi_g(t+1) = \sum_{g'\in G} A_{gg'}\psi_{g'}(t). \tag{3}$$

Unitarity corresponds to the reversibility constraint $\sum_{g'} A_{gg'}A^\dagger_{g''g'} = \sum_{g'} A^\dagger_{gg'}A_{g''g'} = \delta_{gg''}I_{s_g}$.

If we define the set $S_g \subseteq G$ of sites g' interacting with g as the set of sites g' for which $A_{gg'} \neq 0$, the locality requirement amounts to ask that the cardinality of the set S_g is uniformly bounded over G, namely, $|S_g| \leqslant k < \infty$ for every g. In the following we focus on those automata for which, if the transition from g to g' is possible, then also that from g' to g is possible, namely, if $A_{gg'} \neq 0$, then $A_{g'g} \neq 0$.

The homogeneity requirement means that all the sites $g \in G$ are equivalent. In other words, the evolution must not allow one to discriminate two sites g and g'. In mathematical terms, this requirement has three main consequences. The first one is that the cardinality $|S_g|$ is independent of g. The second one is that the set of matrices $\{A_{gg'}\}_{g'\in S_g}$ is the same for every g, whence we will identify the matrices $A_{gg'} = A_h$ for some $h \in S$ with $|S| = |S_g|$. This allows us to define $gh = g'$ if $A_{gg'} = A_h$. In this case, we also formally write $g = g'h^{-1}$. Since for $A_{gg'} \neq 0$ also $A_{g'g} \neq 0$, clearly if $h \in S$ then also $h^{-1} \in S$. The third consequence is that, whenever a sequence of transitions $h_1h_2\cdots h_N$ with $h_i \in S$ connects g to itself, i.e., $gh_1h_2\cdots h_N = g$, then it must also connect any other $g' \in G$ to itself, i.e., $g'h_1h_2\cdots h_N = g'$.

We now define the graph $\Gamma(G,S)$, where the vertices are elements of G, and edges correspond to couples (g,g') with $g' = gh$. The edges can then be colored with $|S|$ colors, in one-to-one correspondence with the transition matrices $\{A_h\}_{h\in S}$. It is now easy to verify that either the graph $\Gamma(G,S)$ is connected or it consists of n disconnected copies of the same connected graph $\Gamma(G_0,S)$. Since the information in G is generally redundant, consisting of n identical and independent copies of the same QCA with cells belonging to G_0, from now on we assume that the graph $\Gamma(G,S)$ is connected. One can now prove that such a graph represents the Cayley graph of a finitely presented group with generators $h \in S$ and relators corresponding to the set R of strings of elements of S corresponding to closed paths. More precisely, we define the free group F of words with letters in S and the free subgroup H generated by words in R; it is easy to check that H is normal in F, thanks to homogeneity. The group G with Cayley graph $\Gamma(G,S)$ coincides with F/N.

In the elementary case there are no self-interactions, and the set S can then be taken as $S = S_+ \cup S_-$, where S_- is the set of inverses of the elements of S_+. In case of self-interactions, we include the identity e in S, which then becomes $S = S_+ \cup S_- \cup \{e\}$. The requirements of unitarity and homogeneity correspond to assuming that the following operator over the Hilbert space $\ell^2(G)\otimes\mathbb{C}^s$ is unitary,

$$A = \sum_{h\in S} T_h \otimes A_h, \tag{4}$$

where T is the right-regular representation of G on $\ell^2(G)$ acting as $T_g|g'\rangle = |g'g^{-1}\rangle$.

Finally, we say that the automaton is isotropic if every direction on $\Gamma(G,S)$ is equivalent. In mathematical terms, there must exist a faithful representation U over $\mathbb{C}^s$ of a group L of graph automorphisms transitive over S_+ such that one has the covariance condition

$$A = \sum_{h\in S} T_h \otimes A_h = \sum_{h\in S} T_{l(h)} \otimes U_l A_h U_l^\dagger, \quad \forall\, l \in L. \tag{5}$$

The existence of such automorphism group implies that the Cayley graph is *symmetric*.

The unitarity conditions in terms of the transition matrices A_h read

$$\begin{gathered} \sum_{h\in S} A_h^\dagger A_h = \sum_{h\in S} A_h A_h^\dagger = I_s, \\ \sum_{\substack{h,h'\in S\\ h^{-1}h'=h''}} A_h^\dagger A_{h'} = \sum_{\substack{h,h'\in S\\ h'h^{-1}=h''}} A_{h'}A_h^\dagger = 0. \end{gathered} \tag{6}$$

In order to have nontrivial sums in the second family of conditions, it is necessary to have generators h_{i_1}, h_{i_2}, h_{i_3}, and h_{i_4} such that, e.g., $h_{i_1}^{-1}h_{i_2}h_{i_4}^{-1}h_{i_3} = e$. In terms of group presentation, this means that the relevant relators for the unitarity conditions are those of length four.

Notice that if the transition matrices $\{A_h\}_{h\in S}$ satisfy the unitarity conditions (6), then also their complex conjugates $\{A_h^*\}_{h\in S}$, their transposes $\{A_{h^{-1}}^T\}_{h\in S}$, and their adjoints $\{A_{h^{-1}}^\dagger\}_{h\in S}$ do, as can be verified taking the complex conjugate, the transpose, or the adjoint of the conditions, and considering that if $h_{i_1}^{-1}h_{i_2} = h_{i_3}^{-1}h_{i_4}$, then also $h_{i_2}^{-1}h_{i_1} = h_{i_4}^{-1}h_{i_3}$.

The QCA in Eq. (5) corresponds to the description of a physical law by a quantum algorithm with finite algorithmic complexity, with homogeneity corresponding to the universality of the law. One can easily recognize the generality of the construction, considering that the group G is abstractly introduced via generators and relators: G can be a random group, have tree-shaped graph, and reflect many other situations. The whole physics will emerge without requiring any metric structure, since the group is defined only topologically. An intuitive notion of metric on the Cayley graph is given by the *word length* $l^w(g)$, defined as $l^w(g) := \min\{n \in \mathbb{N} |\, g = h_{i_1}h_{i_2}\cdots h_{i_n}, h_{i_j} \in S\}$. Space then emerges through the quasi-isometric embedding $\mathsf{E}: G \to R$ of the Cayley graph (Γ, d_Γ) equipped with the *word metric* $d_\Gamma(g,g') = l^w(g^{-1}g')$ in a metric space (R,d_R). Quasi-isometry is defined as [41]

$$\frac{1}{a}d_\Gamma(g,g') - b \leqslant d_R(\mathsf{E}(g),\mathsf{E}(g')) \leqslant a d_\Gamma(g,g') + b, \qquad (7)$$

$$\forall\, x \in R\ \exists g \in G \quad d_R(x,\mathsf{E}(g)) \leqslant c, \qquad (8)$$

for some $a,b,c \in \mathbb{R}$. We also want homogeneity and isotropy to hold locally in the space R; namely, we require for all $g,g' \in G$ and $h,h' \in S$

$$\begin{aligned} d_R(\mathsf{E}(g),\mathsf{E}(gh)) &= d_R(\mathsf{E}(g'),\mathsf{E}(g'h)),\\ d_R(\mathsf{E}(g),\mathsf{E}(gh)) &= d_R(\mathsf{E}(g),\mathsf{E}(gh')). \end{aligned} \qquad (9)$$

The cardinality of group G can be finite or infinite, depending on its relators. The most interesting case in the present context is that of a finitely generated infinite group. Among infinite groups G, we restrict to those having a Cayley graph that is *quasi-isometrically embeddable* [42] in the Euclidean space $\mathbb{R}^d$. Since $\mathbb{R}^d$ and $\mathbb{Z}^d$ are quasi-isometric, every group G that is quasi-isometrically embeddable in $\mathbb{R}^d$ is also quasi-isometric to $\mathbb{Z}^d$. Finally, by the so-called quasi-isometric rigidity of $\mathbb{Z}^d$ every such group G has $\mathbb{Z}^d$ as a subgroup with finitely many cosets; namely, G is *virtually Abelian* of rank d [43].

Our analysis focuses on Abelian groups $\mathbb{Z}^d$.

III. QCAS ON ABELIAN GROUPS

The Cayley graphs of $\mathbb{Z}^d$ satisfying our assumption of isotropic embedding in $\mathbb{R}^d$ are just the Bravais lattices. Since the groups G that we are considering are Abelian, from now on we denote the group elements as usual by boldfaced vector notation as $\mathbf{n} \in G$ and generators as $\mathbf{h} \in S$, and we use the sum notation for the group composition, as well as 0 for the identity. The space $\ell^2(G)$ is the span of $\{|\mathbf{n}\rangle\}_{\mathbf{n}\in G}$ and the right-regular representation coincides with the left-regular. The unitary operator of the automaton is then given by

$$A = \sum_{\mathbf{h}\in S} T_{\mathbf{h}} \otimes A_{\mathbf{h}}, \qquad (10)$$

and one has $[A, T_{\mathbf{h}} \otimes I_s] = 0$. Being the group G Abelian, its unitary irreps are one-dimensional, and are labeled by the joint eigenvectors of $T_{\mathbf{h}}$

$$T_{\mathbf{h}_i}|\mathbf{k}\rangle = e^{-ik_i}|\mathbf{k}\rangle, \qquad (11)$$

where we label the elements $\mathbf{h}_j \in S_+$ by the label j and

$$\mathbf{k} = \sum_{j=1}^{3} k_j \tilde{\mathbf{h}}_j, \qquad (12)$$

where $\tilde{\mathbf{h}}_j \cdot \mathbf{h}_l = \delta_{jl}$. Finally, this implies

$$|\mathbf{k}\rangle = \frac{1}{\sqrt{|B|}}\sum_{\mathbf{n}\in G} e^{-i\mathbf{k}\cdot\mathbf{n}}|\mathbf{n}\rangle, \quad |\mathbf{n}\rangle = \frac{1}{\sqrt{|B|}}\int_B d\mathbf{k}\, e^{i\mathbf{k}\cdot\mathbf{n}}|\mathbf{k}\rangle, \qquad (13)$$

where B is the first Brillouin zone defined through the following set of linear constraints:

$$B := \bigcap_{1\leqslant i\leqslant |S|} \{\mathbf{k} \in \mathbb{R}^d |\, -\pi|\tilde{\mathbf{h}}_i|^2 \leqslant \mathbf{k}\cdot\tilde{\mathbf{h}}_i \leqslant \pi|\tilde{\mathbf{h}}_i|^2\}. \qquad (14)$$

The invariant spaces of the translations T then correspond to plane waves $|\mathbf{k}\rangle$ on the lattice G, with wave vector $\mathbf{k}$. Notice that

$$\langle\mathbf{k}|\mathbf{k}'\rangle = \frac{1}{|B|}\sum_{\mathbf{n}\in G} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{n}} = \delta_B(\mathbf{k}-\mathbf{k}'). \qquad (15)$$

Translation invariance of the automaton in Eq. (10) then implies a form for the unitary operator A,

$$A = \int_B d\mathbf{k} |\mathbf{k}\rangle\langle\mathbf{k}| \otimes \tilde{A}_{\mathbf{k}}, \qquad (16)$$

where $\tilde{A}_{\mathbf{k}} = \sum_{\mathbf{h}\in S} e^{i\mathbf{h}\cdot\mathbf{k}} A_{\mathbf{h}}$ is unitary for every $\mathbf{k}$. Notice that $\tilde{A}_{\mathbf{k}}$ is a matrix polynomial in $e^{i\mathbf{h}\cdot\mathbf{k}}$, as a consequence of the requirement of homogeneity. The spectrum $\{e^{i\omega_{\mathbf{k}}^{(i)}}\}$ of the operator $\tilde{A}_{\mathbf{k}}$ plays a crucial role in the analysis of the dynamics, because the speed of the wave front of a plane wave with wave vector $\mathbf{k}$ is given by the *phase velocity* $\omega_{\mathbf{k}}^{(i)}/|\mathbf{k}|$, while the speed of propagation of a narrowband state having wave vector $\mathbf{k}$ peaked around the value $\mathbf{k}_0$ is given by the *group velocity* at $\mathbf{k}_0$, namely the gradient of the function $\omega_{\mathbf{k}}^{(i)}$ evaluated at $\mathbf{k}_0$. These remarks spot the relevance of the *dispersion relation*, namely the expression of the phases $\omega_{\mathbf{k}}^{(i)}$ as functions of $\mathbf{k}$.

In the $\mathbf{h}$ representation the unitarity conditions (6) for A read

$$\begin{aligned} \sum_{\mathbf{h}\in S} A_{\mathbf{h}}A_{\mathbf{h}}^\dagger &= \sum_{\mathbf{h}\in S} A_{\mathbf{h}}^\dagger A_{\mathbf{h}} = I_s,\\ \sum_{\mathbf{h}-\mathbf{h}'=\mathbf{h}''} A_{\mathbf{h}}A_{\mathbf{h}'}^\dagger &= \sum_{\mathbf{h}-\mathbf{h}'=\mathbf{h}''} A_{\mathbf{h}'}^\dagger A_{\mathbf{h}} = 0. \end{aligned} \qquad (17)$$

In an Abelian group every couple of generators $\mathbf{h},\mathbf{h}'$ is involved at least in one length-four relator expressing Abelianity, namely, $\mathbf{h} - \mathbf{h}' = -\mathbf{h}' + \mathbf{h}$.

In the Abelian case, if $\{A_{\mathbf{h}}\}_{\mathbf{h}\in S}$ is a set of transition matrices satisfying the unitarity conditions (17), in addition to its complex conjugate $\{A^*_{\mathbf{h}}\}_{\mathbf{h}\in S}$, its transpose $\{A^T_{-\mathbf{h}}\}_{\mathbf{h}\in S}$, and its adjoint $\{A^\dagger_{-\mathbf{h}}\}_{\mathbf{h}\in S}$. Also, its reflected set $\{A_{-\mathbf{h}}\}_{\mathbf{h}\in S}$ provides a solution to the conditions (17).

Given an automaton A corresponding to a set of transition matrices $\{A_{\mathbf{h}}\}_{\mathbf{h}\in S}$ satisfying the unitarity condition (17), notice that the identity

$$(I \otimes \tilde{A}^\dagger_{\mathbf{k}=0})A = \sum_{\mathbf{h}\in S} T_{\mathbf{h}} \otimes A'_{\mathbf{h}}, \tag{18}$$

holds, with $\sum_{\mathbf{h}\in S} A'_{\mathbf{h}} = I_s$, namely, modulo a uniform local unitary we can always assume

$$\sum_{\mathbf{h}\in S} A_{\mathbf{h}} = I_s. \tag{19}$$

As explained in Sec. II, the requirement of isotropy for the automaton needs the existence of a group that acts transitively over the generator set S_+ with a faithful representation that satisfies Eq. (5). The isotropy requirement implies that $\tilde{A}_{\mathbf{k}=0}$ commutes with the representation U of the isotropy group L, whence we can classify the automata by requiring identity (19) and then multiplying the operator A on the left by $(I \otimes V)$, with V commuting with the representation U. In the case that U is irreducible, by Schur's lemmas we have only $V = I_s$.

Unitarity of $\tilde{A}_{\mathbf{k}}$ for $s = 1$ amounts to the requirement that, for every $\mathbf{k} \in B$, $|\sum_{\mathbf{h}\in S} z_{\mathbf{h}} e^{i\mathbf{h}\cdot\mathbf{k}}| = 1$ with $z_{\mathbf{h}} \in \mathbb{C}$. This is possible only if $z_{\mathbf{h}} = \delta_{\mathbf{h}_0\mathbf{h}}$ for some generator $\mathbf{h}_0$. However, the only choice of $\mathbf{h}_0$ compatible with isotropy is $\mathbf{h}_0 = 0$, thus providing the trivial automaton $A = I$. From now on we then consider the simplest nontrivial automaton, having $s = 2$.

IV. THE QUANTUM AUTOMATON WITH MINIMAL COMPLEXITY: THE WEYL AUTOMATON

In the present section we solve Eqs. (17) for unitarity, on the Abelian group $\mathbb{Z}^3$.

For $d = 3$, the only Cayley graphs are the primitive cubic (PC) lattice corresponding to the presentation of $\mathbb{Z}^3$ as the free Abelian group on d generators, the bcc, corresponding to a presentation with four generators $S_+ = \{\mathbf{h}_i\}_{1\leqslant i\leqslant 4}$ with relator $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$, and the rhombohedral, having six generators $S_+ = \{\mathbf{h}_i\}_{1\leqslant i\leqslant 6}$ with relators $\mathbf{h}_1 - \mathbf{h}_2 = \mathbf{h}_4$, $\mathbf{h}_2 - \mathbf{h}_3 = \mathbf{h}_5$, and $\mathbf{h}_3 - \mathbf{h}_1 = \mathbf{h}_6$. The corresponding coordination numbers are 6, 8, and 12, respectively (notice that the other Bravais lattices are topologically equivalent to the above three ones; namely, they are the same lattice modulo stretching transformations that do not change the graph). The unitarity conditions are very restrictive and allow for a solution only on one of three possible Cayley graphs for $\mathbb{Z}^3$. Moreover, the automata satisfying our principles are only four, modulo unitary conjugation. The solutions are divided in two pairs, $A^\pm$ and $B^\pm$. A pair of solutions is connected to the other pair by transposition in the canonical basis, i.e., $\tilde{A}^\pm_{\mathbf{k}} = (\tilde{B}^\pm_{\mathbf{k}})^T$.

We call these solutions Weyl automata, because in the relativistic limit of small wave-vector $|\mathbf{k}| \ll 1$ their evolution obeys Weyl's equation, as discussed in Sec. VII.

In Appendix A the details of the derivation are explained, along with the proof of impossibility for a QCA on the PC and rhombohedral lattices.

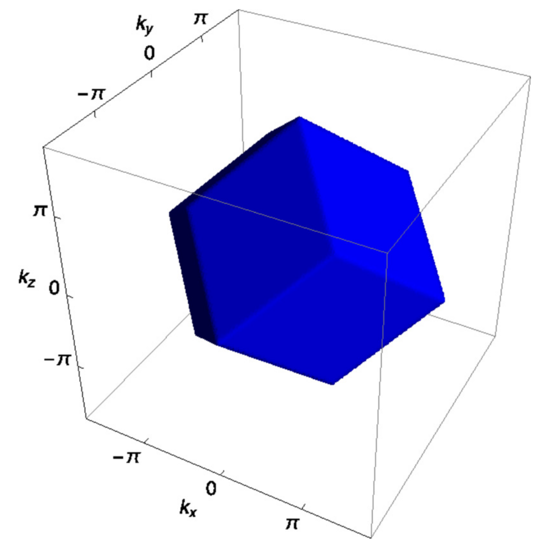

FIG. 1. (Color online) The Brillouin zone for the bcc lattice. The components of the wave vector $\mathbf{k}$ are dimensionless.

Let us now describe the bcc lattice in more detail. The corresponding presentation of $\mathbb{Z}^3$ involves four vectors, $S_+ = \{\mathbf{h}_1,\mathbf{h}_2,\mathbf{h}_3,\mathbf{h}_4\}$, with relator $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$. The four vectors can be chosen as follows:

$$\begin{aligned} \mathbf{h}_1 &= \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}, \quad \mathbf{h}_2 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\-1\\-1\end{pmatrix}, \\ \mathbf{h}_3 &= \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\1\\-1\end{pmatrix}, \quad \mathbf{h}_4 = \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\-1\\1\end{pmatrix}. \end{aligned} \tag{20}$$

The 12 dual vectors $\tilde{k}_i$ satisfying $\mathbf{h}_i \cdot \tilde{\mathbf{h}}_j = \delta_{ij}$ are

$$\tilde{\mathbf{h}} = \frac{\sqrt{3}}{2}\begin{pmatrix}1\\\pm1\\0\end{pmatrix}, \tag{21}$$

modulo permutations of the three components and an overall sign. The Brillouin zone for the bcc lattice—shown in Fig. 1—is defined by

$$B := \left\{\mathbf{k}\middle| -\frac{3\pi}{2} \leqslant \mathbf{k}\cdot\tilde{\mathbf{h}}_i \leqslant \frac{3\pi}{2}, 1 \leqslant i \leqslant 6\right\}, \tag{22}$$

which in Cartesian coordinates, using Eq. (21), reads

$$-\sqrt{3}\pi \leqslant k_i \pm k_j \leqslant \sqrt{3}\pi, \quad i \neq j \in \{x,y,z\}. \tag{23}$$

Two solutions $A^\pm$ of the unitarity equations correspond to the following transition matrices $A_{\mathbf{h}_i}$:

$$\begin{aligned} A_{\mathbf{h}_1} &= \begin{pmatrix}\zeta^* & 0\\ \zeta^* & 0\end{pmatrix}, \quad A_{-\mathbf{h}_1} = \begin{pmatrix}0 & -\zeta\\ 0 & \zeta\end{pmatrix}, \\ A_{\mathbf{h}_2} &= \begin{pmatrix}0 & \zeta^*\\ 0 & \zeta^*\end{pmatrix}, \quad A_{-\mathbf{h}_2} = \begin{pmatrix}\zeta & 0\\ -\zeta & 0\end{pmatrix}, \\ A_{\mathbf{h}_3} &= \begin{pmatrix}0 & -\zeta^*\\ 0 & \zeta^*\end{pmatrix}, \quad A_{-\mathbf{h}_3} = \begin{pmatrix}\zeta & 0\\ \zeta & 0\end{pmatrix}, \\ A_{\mathbf{h}_4} &= \begin{pmatrix}\zeta^* & 0\\ -\zeta^* & 0\end{pmatrix}, \quad A_{-\mathbf{h}_4} = \begin{pmatrix}0 & \zeta\\ 0 & \zeta\end{pmatrix}. \end{aligned} \tag{24}$$

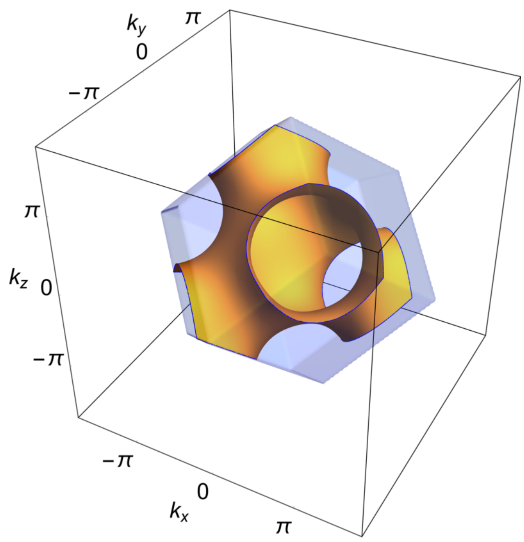

FIG. 2. (Color online) Plot of the surface $\omega_{\mathbf{k}}^{A^+} = \frac{\pi}{2}$ within the Brillouin zone for the bcc lattice. The components of the wave vector $\mathbf{k}$ are dimensionless.

The remaining solutions are the transposes $\tilde{B}_{\mathbf{k}}^{\pm} = (\tilde{A}_{\mathbf{k}}^{\pm})^T$. As we will see later, the solutions $\tilde{B}_{\mathbf{k}}^{\pm}$ are redundant.

The solutions $A_{\mathbf{k}}^{\pm}$ in the Fourier representation are

$$\begin{aligned} \tilde{A}_{\mathbf{k}}^{\pm} &= \frac{1}{4}\begin{pmatrix} z(\mathbf{k}) & -w(\mathbf{k})^* \\ w(\mathbf{k}) & z(\mathbf{k})^* \end{pmatrix}, \\ z(\mathbf{k}) &:= \zeta^* e^{ik_1} + \zeta e^{-ik_2} + \zeta e^{-ik_3} + \zeta^* e^{ik_4}, \\ w(\mathbf{k}) &:= \zeta^* e^{ik_1} + \zeta e^{-ik_2} - \zeta e^{-ik_3} - \zeta^* e^{ik_4}, \\ \zeta &= \frac{1 \pm i}{4}, \end{aligned} \tag{25}$$

and can be written as

$$\tilde{A}_{\mathbf{k}}^{\pm} = I d_{\mathbf{k}}^{A^{\pm}} - i\boldsymbol{\alpha}^{\pm} \cdot \mathbf{a}_{\mathbf{k}}^{A^{\pm}}, \tag{26}$$

where we define

$$\begin{aligned} \left(a_{\mathbf{k}}^{A^{\pm}}\right)_x &:= s_x c_y c_z \pm c_x s_y s_z, \\ \left(a_{\mathbf{k}}^{A^{\pm}}\right)_y &:= c_x s_y c_z \mp s_x c_y s_z, \\ \left(a_{\mathbf{k}}^{A^{\pm}}\right)_z &:= c_x c_y s_z \pm s_x s_y c_z, \\ d_{\mathbf{k}}^{A^{\pm}} &:= c_x c_y c_z \mp s_x s_y s_z. \end{aligned} \tag{27}$$

The symbols c_i and s_i denote $\cos\frac{k_i}{\sqrt{3}}$ and $\sin\frac{k_i}{\sqrt{3}}$, respectively, while $\boldsymbol{\alpha}^{\pm}$ is the vector of matrices

$$\alpha_x^{\pm} := \sigma_x, \quad \alpha_y^{\pm} := \mp\sigma_y, \quad \alpha_z^{\pm} := \sigma_z. \tag{28}$$

As one can see from (26), the matrices $\tilde{A}_{\mathbf{k}}^{\pm}$ have unit determinant, with spectrum $\{e_{\mathbf{k}}^{-i\omega^{A^{\pm}}}, e_{\mathbf{k}}^{i\omega^{A^{\pm}}}\}$, and the dispersion relation is given by

$$\omega_{\mathbf{k}}^{A^{\pm}} = \arccos(c_x c_y c_z \mp s_x s_y s_z). \tag{29}$$

In Fig. 2 a plot lot of the surface $\omega_{A^+} = \frac{\pi}{2}$ within the Brillouin zone is given.

The three vectors that rule the evolution are (i) the wave vector $\mathbf{k}$, (ii) the helicity direction $\mathbf{a}_{\mathbf{k}}^{A^{\pm}}$, and (iii) the group velocity $\mathbf{v}_{\mathbf{k}}^{\pm} := \nabla_{\mathbf{k}}\omega_{\mathbf{k}}^{\pm}$, representing the speed of a wave packet peaked around the central wave vector $\mathbf{k}$. The group velocity has the components

$$\left(v_{\mathbf{k}}^{A^{\pm}}\right)_x = \frac{\left(a_{\mathbf{k}}^{A^{\pm}}\right)_x}{\sqrt{1-\left(d_{\mathbf{k}}^{A^{\pm}}\right)^2}}, \tag{30}$$

$$\left(v_{\mathbf{k}}^{A^{\pm}}\right)_y = \frac{\left(a_{\mathbf{k}}^{A^{\mp}}\right)_y}{\sqrt{1-\left(d_{\mathbf{k}}^{A^{\pm}}\right)^2}}, \tag{31}$$

$$\left(v_{\mathbf{k}}^{A^{\pm}}\right)_z = \frac{\left(a_{\mathbf{k}}^{A^{\pm}}\right)_z}{\sqrt{1-\left(d_{\mathbf{k}}^{A^{\pm}}\right)^2}}, \tag{32}$$

where we remark the sign mismatch for the y component. An alternate, convenient expression of the two automata above is the following:

$$\tilde{A}_{\mathbf{k}}^{\pm} = e^{-i\frac{k_x}{\sqrt{3}}\sigma_x} e^{\mp i\frac{k_y}{\sqrt{3}}\sigma_y} e^{-i\frac{k_z}{\sqrt{3}}\sigma_z}. \tag{33}$$

If we now consider the automata $\tilde{A}_{\mathbf{k}}^{\pm}$ and translate their argument as $\mathbf{k}' := \mathbf{k} + \frac{\sqrt{3}\pi}{2}\mathbf{k}_i$ along the directions $\mathbf{k}_0 := (1,1,1)$, $\mathbf{k}_1 := (1,-1,-1)$, $\mathbf{k}_2 := (-1,1,-1)$, or $\mathbf{k}_3 := (-1,-1,1)$, we obtain $\tilde{A}_{\mathbf{k}'}^{\pm} = \mp\tilde{B}_{\mathbf{k}}^{\mp}$. Similarly, if we translate in the same way along the directions $-\mathbf{k}_0$, $-\mathbf{k}_1$, $-\mathbf{k}_2$, or $-\mathbf{k}_3$, we obtain $\tilde{A}_{\mathbf{k}'}^{\pm} = \pm\tilde{B}_{\mathbf{k}}^{\mp}$. Finally, if we translate by $\sqrt{3}\pi$ along the Cartesian axes, we obtain $\tilde{A}_{\mathbf{k}'}^{\pm} = -\tilde{A}_{\mathbf{k}}^{\pm}$.

One can easily verify that the two automata $\tilde{A}_{\mathbf{k}}^{\pm}$ are covariant under the group L_2 of binary rotations around the coordinate axes, with the representation of the group L_2 on $\mathbb{C}^2$ given by $\{I, i\sigma_x, i\sigma_y, i\sigma_z\}$.

Finally, the two automata are connected by the following identity:

$$\tilde{A}_{\mathbf{k}}^{\pm} = \tilde{A}_{-\mathbf{k}}^{\mp *}. \tag{34}$$

Since for $\mathbb{SU}(2)$ matrices complex conjugation is obtained unitarily by conjugation with σ_y, the essential connection between the two solutions $\tilde{A}_{\mathbf{k}}^{\pm}$ is a parity reflection $P : \mathbf{k} \mapsto -\mathbf{k}$.

Summarizing, we can say that the automata $A^{\pm}$ and $A^{\mp *}$ are connected by the P symmetry, $A^{\pm}$ and $B^{\pm *}$ by the T symmetry, and $A^{\pm}$ and $B^{\mp}$ by PT symmetry. Charge conjugation for the Weyl automata is not defined.

V. COUPLING WEYL AUTOMATA: THE DIRAC AUTOMATA

In this section we find the only two automata that can be obtained by locally coupling Weyl automata. These automata are called Dirac automata, because in the relativistic limit of $|\mathbf{k}| \ll 1$ they give Dirac's equation, a discussed in Sec. VII.

We start from two arbitrary Weyl automata F and D, which can be $A^{\pm}$ or $B^{\pm}$. The coupling is obtained by performing the direct sum of their representatives $\tilde{F}_{\mathbf{k}}$ and $\tilde{D}_{\mathbf{k}}$, obtaining a QCA with $s = 4$ and introducing off-diagonal blocks B and C in such a way that the obtained matrix is unitary. Locality of the coupling requires the off-diagonal blocks B and C to be independent of $\mathbf{k}$, namely,

$$\tilde{A}'_{\mathbf{k}} := \begin{pmatrix} x\tilde{F}_{\mathbf{k}} & yB \\ zC & t\tilde{D}_{\mathbf{k}} \end{pmatrix}, \tag{35}$$

where x and t are generally complex, whereas y and z can be chosen as positive. In Appendix B the derivation is carried out, leading to the only two possible automata,

$$\tilde{E}^{\pm}_{\mathbf{k}} := \begin{pmatrix} n\tilde{A}^{\pm}_{\mathbf{k}} & imI \\ imI & n\tilde{A}^{\pm\dagger}_{\mathbf{k}} \end{pmatrix}, \tag{36}$$

with $n^2 + m^2 = 1$.

Notice also that the choice of $B^{\pm}$ instead of $A^{\pm}$ would have led to a unitarily equivalent automaton, since $\tilde{B}^{\pm *}_{\mathbf{k}} = \sigma_y \tilde{B}^{\pm}_{\mathbf{k}} \sigma_y = \tilde{A}^{\pm\dagger}_{\mathbf{k}}$, and the exchange of the upper left block with the lower right one can be achieved unitarily.

The eigenvalues $\{\lambda^{E^{\pm}}_{\mathbf{k}}, \lambda^{E^{\pm}*}_{\mathbf{k}}\}$ of $\tilde{E}_{\mathbf{k}}$ are derived in Appendix B along with the projections on the eigenspaces, and their expression $\lambda^{E^{\pm}}_{\mathbf{k}} = e^{-i\omega^{E^{\pm}}_{\mathbf{k}}}$ is given in terms of the following dispersion relation:

$$\omega^{E^{\pm}}_{\mathbf{k}} = \arccos[\sqrt{1-m^2}(c_x c_y c_z \mp s_x s_y s_z)]. \tag{37}$$

The Dirac automaton can be expressed in terms of the γ matrices in the spinorial representation as

$$\tilde{E}^{\pm}_{\mathbf{k}} = I d^{E\pm}_{\mathbf{k}} - i\gamma^0 \boldsymbol{\gamma}^{\pm} \cdot \mathbf{a}^{E\pm}_{\mathbf{k}} + im\gamma^0, \tag{38}$$

where $d^{E\pm} = nd^{A\pm}$ and $\mathbf{a}^{E\pm} = n\mathbf{a}^{A\pm}$. The representations $\boldsymbol{\gamma}^{\pm}$ only differ by a sign on γ^2.

Notice that the two automata E^+ and E^- are connected by a CPT symmetry, modulo the unitary transformation $\gamma^0\gamma^2$, where the CPT transformations are defined here by C (charge conjugation): $C: \tilde{E}_{\mathbf{k}} \mapsto -\gamma^2 \tilde{E}^*_{\mathbf{k}} \gamma^2$, $P: \mathbf{k} \mapsto -\mathbf{k}$, and $T: E \mapsto E^{\dagger}$.

VI. THE DIRAC AUTOMATON IN ONE AND TWO SPACE DIMENSIONS

In this section we show the solution to the unitarity conditions in Eq. (6) on Cayley graphs of $\mathbb{Z}$ and $\mathbb{Z}^2$.

A. Two-dimensional case

For $d = 2$, the only Cayley graphs that are topologically inequivalent are the square lattice corresponding to the presentation of $\mathbb{Z}^2$ as the free Abelian group on two generators and the hexagonal lattice, corresponding to a presentation with three generators $S_+ = \{\mathbf{h}_i\}_{1\leqslant i\leqslant 3}$ with relator $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 = 0$. The corresponding coordination numbers are 4 and 6, respectively. Analogously to the case $d = 3$, also for $d = 2$ the unitarity conditions allow for a solution only on one of the possible Cayley graphs, precisely the square lattice. In this case there are only two solutions modulo unitary conjugation, and they are connected by transposition. In the relativistic limit of small wave vector $|\mathbf{k}| \ll 1$ their evolution obeys Weyl's equation in $d = 2$, as discussed in Sec. VII.

Since the second solution is just the transpose of the first one, only the first solution is derived in Appendix C and corresponds to an expression for the automaton,

$$\begin{aligned}
\tilde{A}_{\mathbf{k}} &= \frac{1}{4}\begin{pmatrix} z(\mathbf{k}) & iw(\mathbf{k})^* \\ iw(\mathbf{k}) & z(\mathbf{k})^* \end{pmatrix}, \\
z(\mathbf{k}) &:= \zeta^*(e^{ik_1} + e^{-ik_1}) + \zeta(e^{ik_2} + e^{-ik_2}) \\
w(\mathbf{k}) &:= \zeta(e^{ik_1} - e^{-ik_1}) + \zeta^*(e^{ik_2} - e^{-ik_2}) \\
\zeta &:= \frac{1+i}{4},
\end{aligned} \tag{39}$$

which can be written as

$$\tilde{A}_{\mathbf{k}} = I d^A_{\mathbf{k}} - i\boldsymbol{\alpha} \cdot \mathbf{a}^A_{\mathbf{k}}, \tag{40}$$

where $\alpha_i := \sigma_i$ and the functions $\mathbf{a}_{\mathbf{k}}$ and $d_{\mathbf{k}}$ are expressed in terms of $k_x := \frac{k_1+k_2}{\sqrt{2}}$ and $k_y := \frac{k_1-k_2}{\sqrt{2}}$ as

$$\begin{aligned}
\left(a^A_{\mathbf{k}}\right)_x &:= s_x c_y, & \left(a^A_{\mathbf{k}}\right)_y &:= c_x s_y, \\
\left(a^A_{\mathbf{k}}\right)_z &:= s_x s_y, & d^A_{\mathbf{k}} &:= c_x c_y.
\end{aligned} \tag{41}$$

The symbols c_i and s_i denote $\cos\frac{k_i}{\sqrt{2}}$ and $\sin\frac{k_i}{\sqrt{2}}$, respectively.

The dispersion relation is

$$\omega^A_{\mathbf{k}} = \arccos(c_x c_y); \tag{42}$$

then the helicity vector is $\mathbf{a}^A_{\mathbf{k}}$, and the group velocity is then

$$\left(v^A_{\mathbf{k}}\right)_x = \frac{\left(a^A_{\mathbf{k}}\right)_x}{\sqrt{1 - \left(d^A_{\mathbf{k}}\right)^2 - \left(a^A_{\mathbf{k}}\right)_z^2}}, \tag{43}$$

$$\left(v^A_{\mathbf{k}}\right)_y = \frac{\left(a^{A\mp}_{\mathbf{k}}\right)_y}{\sqrt{1 - \left(d^A_{\mathbf{k}}\right)^2 - \left(a^A_{\mathbf{k}}\right)_z^2}}. \tag{44}$$

The QCA in Eq. (39) is covariant for the cyclic transitive group $L = \{e, a\}$ generated by the transformation a that exchanges $\mathbf{h}_1$ and $\mathbf{h}_2$, with representation given by the rotation by π around the x axis.

Since the isotropy group has a reducible representation, the most general automaton is actually given by

$$(\cos\theta I + i\sin\theta\sigma_x)\tilde{A}_{\mathbf{k}}. \tag{45}$$

However, the parameter θ in this case just represents a fixed translation of the Brillouin zone along the k_x direction, namely a redefinition of the wave vector. The physics is essentially independent of θ, and it is then safe to restrict to $\tilde{A}_{\mathbf{k}}$.

The other solution B can be simply obtained by taking $\tilde{B}_{\mathbf{k}} := \tilde{A}^T_{\mathbf{k}}$.

The only possible automaton describing a local coupling of two Weyl's is obtained by the same procedure as for the three-dimensional (3D) case, described in Appendix B, and is given by

$$\tilde{E}_{\mathbf{k}} = \begin{pmatrix} n\tilde{A}_{\mathbf{k}} & imI \\ imI & n\tilde{A}^{\dagger}_{\mathbf{k}} \end{pmatrix}, \tag{46}$$

with $n^2 + m^2 = 1$.

As in the 3D case, we can write the automaton $\tilde{E}_{\mathbf{k}}$ in terms of the γ matrices as

$$\tilde{E}_{\mathbf{k}} = I d^E_{\mathbf{k}} - i\gamma^0 \boldsymbol{\gamma} \cdot \mathbf{a}^E_{\mathbf{k}} + im\gamma^0, \tag{47}$$

where $d^E_{\mathbf{k}} = nd^A_{\mathbf{k}}$ and $\mathbf{a}^E_{\mathbf{k}} = n\mathbf{a}^A_{\mathbf{k}}$.

B. One-dimensional case

For the sake of completeness, we consider the 1D case studied in Refs. [14,44], rephrasing it in in the present framework.

The unique Cayley graph satisfying our requirements for $\mathbb{Z}$ is the lattice $\mathbb{Z}$ itself, presented as the free Abelian group on one generator. In this case the nearest neighbors are two. The unitarity conditions for a Weyl spinor then read

$$A^{\dagger}_{\mathbf{h}} A_{-\mathbf{h}} = A_{\mathbf{h}} A^{\dagger}_{-\mathbf{h}} = 0, \tag{48}$$

and, consequently,

$$A_{\mathbf{h}} = VM, \quad A_{-\mathbf{h}} = V(I - M), \tag{49}$$

where M is a rank 1 projection that we identify with the eigenspace of σ_z with eigenvalue -1. We then have

$$\tilde{A}_k^{(1)} = \begin{pmatrix} e^{-ik} & 0 \\ 0 & e^{ik} \end{pmatrix}. \tag{50}$$

This matrix can be expressed as

$$d_k^{(1)} I - i a_k^{(1)} \alpha^{(1)}, \tag{51}$$

where $\alpha^{(1)} := \sigma_z$ and

$$d_k^{(1)} := \cos k, \quad a_k^{(1)} := \sin k. \tag{52}$$

The dispersion relation is simply

$$\omega_k^{A^{(1)}} = k. \tag{53}$$

Modulo a permutation of the canonical basis, the coupling of two conjugate Weyl spinors is obtained as in Appendix B, and for $d = 1$ gives two independent $s = 2$ automata as

$$\tilde{E}_k^{(1)} = \begin{pmatrix} ne^{-ik} & im & 0 & 0 \\ im & ne^{ik} & 0 & 0 \\ 0 & 0 & ne^{ik} & im \\ 0 & 0 & im & ne^{-ik} \end{pmatrix}, \tag{54}$$

both having dispersion relation

$$\omega_k^{E^{(1)}} = \arccos(n \cos k). \tag{55}$$

In this case we can express each of the two spinor automata in terms of the Pauli matrices as

$$\tilde{E}_k^{(1)} = n \cos k I - in \sin k \sigma_z + im\sigma_x. \tag{56}$$

VII. THE RELATIVISTIC LIMIT

In the present section we study the behavior of the automata studied in the previous sections for small wave vectors $|\mathbf{k}| \ll 1$. The physical domain in which this limit applies is strictly related to the hypotheses that we make on the order of magnitude of the lattice step and of the time step of the automata. As we discussed in the Introduction, our assumption is that automata describe physics at a discrete Planck scale, which amounts to taking the time step steps equal to the Planck time t_P in dimensionful units. Moreover, as we see in the following, we recover Weyl's and Dirac's equations in the mentioned limit, with the speed of light replaced with a constant speed $c = a/(\sqrt{d} t_P)$, where a is the length of the lattice step. If we want c equal to the speed of light, then we must take the lattice step a as $a = \sqrt{d} l_P$, where l_P is the Planck length. Having set these conversion factors between dimensionless and dimensionful units, the limit of $|\mathbf{k}| \ll 1$ corresponds to the limit where wavelengths $\lambda = 1/|\mathbf{k}|$ are much larger than the Planck length. This clearly encompasses all the relativistic regimes tested in most advanced experiments in high-energy physics.

In order to obtain the relativistic limit of the automata studied in the previous sections, we define an *interpolating Hamiltonian* $H_I^X(\mathbf{k})$ as

$$e^{-iH_I^X(\mathbf{k})} := \tilde{X}_{\mathbf{k}}, \tag{57}$$

for any of the automata $X = \tilde{A}_{\mathbf{k}}^{\pm}, \tilde{B}_{\mathbf{k}}^{\pm}, \tilde{A}_{\mathbf{k}}, \tilde{B}_{\mathbf{k}}, \tilde{A}_{\mathbf{k}}^{(1)}, \tilde{E}_{\mathbf{k}}^{\pm}, \tilde{E}_{\mathbf{k}}, \tilde{E}_{\mathbf{k}}^{(1)}$ studied in the previous sections. The term *interpolating* refers to the fact that the Hamiltonian $H_I^X(\mathbf{k})$ generates a unitary evolution that interpolates the discrete time determined by the automaton steps through a continuous time t as

$$\psi(\mathbf{k},t) = e^{-iH_I^X(\mathbf{k})t} \psi(\mathbf{k},0). \tag{58}$$

In the case of Weyl automata, independently of the dimension d, for narrowband states $\psi(\mathbf{k},t)$ with $|\mathbf{k}| \ll 1$, expanding of $H_I^X(\mathbf{k})$ to the first order in $\mathbf{k}$ we obtain

$$i\partial_t \psi(\mathbf{k},t) = H_W^X(\mathbf{k})\psi(\mathbf{k},t), \tag{59}$$

where $H_W(\mathbf{k})$ is the Weyl Hamiltonian, obtained by expanding $H_F^X(\mathbf{k})$ to first order in $\mathbf{k}$, namely,

$$H_W^X(\mathbf{k}) = \frac{1}{\sqrt{d}} \boldsymbol{\alpha}^X \cdot \mathbf{k} + O(|\mathbf{k}|^2). \tag{60}$$

Similarly, in the case of the Dirac automata, for narrowband states $\psi(\mathbf{k},t)$ with $|\mathbf{k}| \ll 1$ the expansion of $H_I^X(\mathbf{k})$ to the first order in $\mathbf{k}$ gives

$$i\partial_t \psi(\mathbf{k},t) = H_D(\mathbf{k})\psi(\mathbf{k},t), \tag{61}$$

where $H_D(\mathbf{k})$ is the Dirac Hamiltonian, obtained by expanding $H_E(\mathbf{k})$ at first order in $\mathbf{k}$, namely,

$$H_D(\mathbf{k}) = \frac{n}{\sqrt{d}} \boldsymbol{\alpha} \cdot \mathbf{k} + m\beta + O(|\mathbf{k}|^2). \tag{62}$$

Finally, for small values of m, $m \ll 1$, we have $n \simeq 1 + O(m^2)$. Neglecting terms of order $O(m^2)$ and $O(|\mathbf{k}|^2)$, we then get

$$H_D(\mathbf{k}) = \frac{1}{\sqrt{d}} \boldsymbol{\alpha} \cdot \mathbf{k} + m\beta, \tag{63}$$

which is the Dirac equation in the wave-vector representation. Notice that in the case of the $\tilde{E}_{\mathbf{k}}^{-}$ automaton in 3D the Dirac Hamiltonian is recovered in the spinorial representation where the complex conjugate of γ^2 is taken instead of γ^2.

In Fig. 3 we show two samples of the evolution of the 2D Dirac automaton are given, for a localized state and a particlelike state.

We now provide a quantitative study of the approximation of Dirac's equation in 3D in the relativistic limit of $|\mathbf{k}| \ll 1$, $m \ll 1$ $[O(m) = O(|\mathbf{k}|)]$. First we compare the automaton with the Dirac equation in dimensionless units with dispersion relation $\omega^E(\mathbf{k}) = (m^2 + \frac{k^2}{6})^{\frac{1}{2}}$, and then we recover the usual Dirac equation with dispersion $\hbar\omega^D(\mathbf{p}) := (m^2c^4 + c^2p^2)^{\frac{1}{2}}$ by introducing dimensions for the automaton time and lattice steps. We compare the two evolutions for a particle state in a fixed spin state, with a narrow packet around $\mathbf{k}_0 \ll 1$, with variance $\sigma \ll |\mathbf{k}_0|$. The trace-norm distance between the output states from the same input state evolved under the Dirac Hamiltonian and under the automaton, respectively, is given by $\sqrt{1 - F^2}$, where F is the fidelity between the two states, which is given by $F = |\langle \exp[-iN\Delta(\mathbf{k})]\rangle|$, where N is the number of steps of the automaton (each corresponding to a Planck time for the Dirac evolution, or equivalently to an integer time for a Dirac equation written in dimensionless form in Planck units), the expectation is over the input state, and the operator $\Delta(\mathbf{k}) := (m^2 + \frac{k^2}{6})^{\frac{1}{2}} - \omega^E(\mathbf{k})$, diagonal in the eigenbasis of

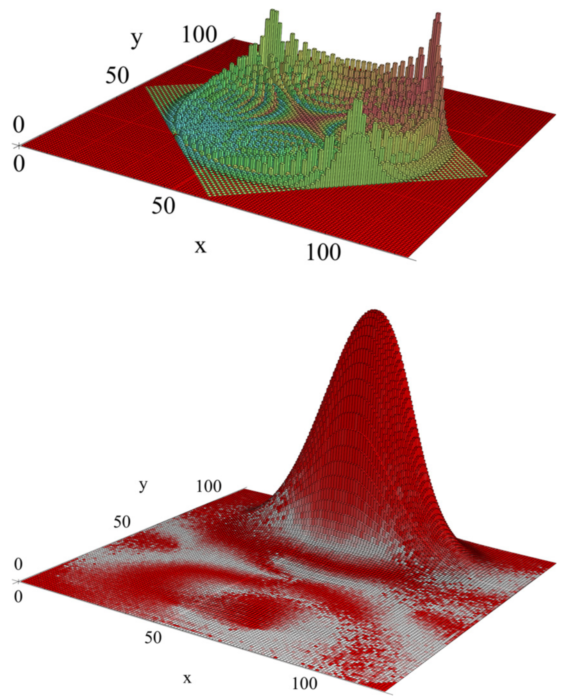

FIG. 3. (Color online) Examples of evolution of for the 2D Dirac automaton for $m = 0.1$, $N = 120$, corresponding to coupling of two Weyl's in Eq. (C21) for (top) $|\langle \mathbf{x}| \otimes \langle \mathbf{e}_1|\psi(0)\rangle|^2$ and $\psi(0)$ localized in $\mathbf{x} = 0$ in state $|\mathbf{e}_1\rangle$ ($|\mathbf{e}_n\rangle$, $n = 1,\ldots,4$ canonical basis i $\mathbb{C}^4$) and (bottom) $|\langle \mathbf{x}| \otimes \langle \mathbf{u}_1(\mathbf{k})|\psi(0)\rangle|^2$ for $|\psi(0)\rangle$ Gaussian spin-up particle state with $\mathbf{k}_0 = (0,.1)\pi$ centered in $\mathbf{x} = 0$ with $\Delta_x^2 = 10^2$, $\Delta_y^2 = 50$, with $|\mathbf{u}_1(\mathbf{k})\rangle$ denoting the spin-up component of the particle eigenvector. The color code corresponds to the spin-component relative weight (hue) and relative phase (saturation). Notice the colored square with vanishing small probability, corresponding to the causal velocity, which is $\sqrt{2}$ times larger than the propagation speed. The coordinates x and y are dimensionless, the unit being the lattice step.

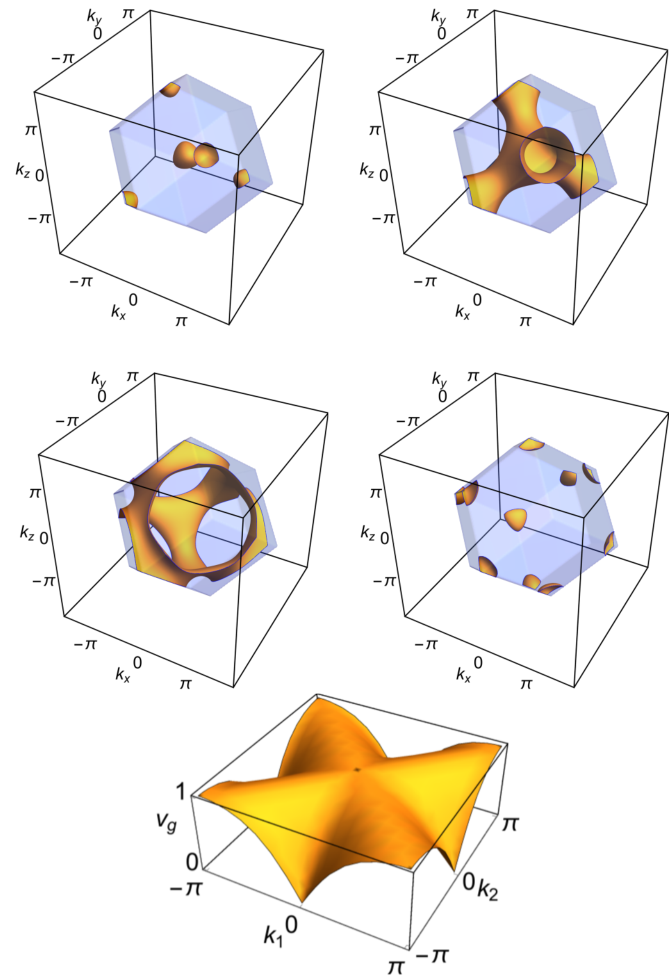

FIG. 4. (Color online) (Top) Dispersion relation $\omega_{\mathbf{k}}^{E^+}$ for the 3D Dirac automaton for $m = 0$ and for $\omega_{\mathbf{k}}^{E^+} = 0.45, 1.05, 2.09, 2.69$ from left to right. (Bottom) modulus of group velocity $\mathbf{v_k} = \nabla_{\mathbf{k}}\omega(\mathbf{k})$ for the 2D case for $m = 0$. The components of the wave vector $\mathbf{k}$ are dimensionless.

the Dirac Hamiltonian to the order $O(k^4 + N^{-1}k^2)$, is given by

$$\Delta(\mathbf{k}) = \frac{\sqrt{3}k_xk_yk_z}{\left(m^2 + \frac{k^2}{3}\right)^{\frac{1}{2}}} - \frac{3(k_xk_yk_z)^2}{\left(m^2 + \frac{k^2}{3}\right)^{\frac{3}{2}}} + \frac{1}{24}\left(m^2 + \frac{k^2}{3}\right)^{\frac{3}{2}},$$

where the term $O(N^{-1}k^2)$ comes from the mismatch between the eigenvectors of the automaton and the Dirac particle states. One can see the the fidelity approaches $F = 1$ in the relativistic limit, for not too large a number of steps. In the relativistic scale $k \simeq m \ll 1$, for a proton mass one has $N \simeq m^{-3} = 2.2 \times 10^{57}$, corresponding to $t = 1.2 \times 10^{14}$ s $= 3.7 \times 10^6$ y. The approximation is still good in the ultrarelativistic case $k \gg m$, e.g., for $k = 10^{-8}$ (as for ultra-high energy cosmic rays), where it holds for $N \simeq k^{-2} = 10^{16}$ steps, corresponding to 5×10^{-28} s. We convert dimensionless to dimensionful quantities through the Planck units l_P, m_P, and t_P as

$$c := l_P/t_P, \quad \mu := mm_P, \quad \hbar := m_Pl_Pc, \quad p = \hbar k/(\sqrt{3}l_P), \tag{64}$$

where c is the speed of light, μ the rest mass, and p the momentum. The above choice corresponds to taking m_P as the bound for rest mass of the particle, l_P as half of the side of the conventional bcc cell, and t_P as the time of a single automaton step. Upon substituting Eq. (64) one can immediately check that $\omega^E(\mathbf{k}) = t_P\omega^D(\mathbf{p})$. One can also see that the speed of light c is slower than the causal speed—i.e., one site per Planck time—by a factor $\sqrt{3}$. Indeed, isotropy is recovered only in the relativistic limit: At the Planck scale there is a possibility of propagation at speed higher than c, however, bounded by $\sqrt{3}c$ and with a negligible probability, as shown in Fig. 3. Notice that a similar analysis holds also for $d = 1,2$, and the rescaling factor in the general case is $\sqrt{d}$. In Fig. 4 we report the dispersion relation for the Dirac automaton for $d = 2,3$ with $m = 0$. In the 3D dispersion relation, in addition to the central ball in the rightmost figure, corresponding to the usual particle dispersion, one can notice four balls corresponding to the so-called Fermion doubling [45,46]. The plot of the group velocity of the 2D automaton exhibits anisotropy; however, the flat central area incorporates huge ultrarelativistic moments with velocity still perfectly isotropic.

For narrowband states around $\mathbf{k} = \mathbf{k}_0$ we can approximate the automaton evolution also in the Planck regime with a dispersive Schrödinger equation,

$$i\partial_t \tilde{\psi}(\mathbf{x},t) = \pm\left[\mathbf{v}\cdot\nabla + \tfrac{1}{2}\mathbf{D}\cdot\nabla\nabla\right]\tilde{\psi}(\mathbf{x},t), \tag{65}$$

where $\tilde{\psi}(\mathbf{x},t)$ is the Fourier transform of $\tilde{\psi}(\mathbf{k},t) := e^{-i\mathbf{k}_0\cdot\mathbf{x}+i\omega_0 t}\psi(\mathbf{k},t)$, and $\mathbf{v}$ and $\mathbf{D}$ are the drift vector $\mathbf{v} = (\nabla_{\mathbf{k}}\omega)(\mathbf{k}_0)$ and diffusion tensor $\mathbf{D} = (\nabla_{\mathbf{k}}\nabla_{\mathbf{k}}\omega)(\mathbf{k}_0)$, respectively. The Schrödinger equation is just the second-order $\mathbf{k}$ expansion around $\mathbf{k}_0$. This equation approximates well the evolution, also in the Planck regime for many steps, depending on the bandwidth (see Ref. [44]).

VIII. CONCLUSION

We introduced a representation of space as emergent from the evolution of quantum systems via a QCA and imposed the principles of unitarity, linearity, locality, homogeneity, and isotropy of the evolution, showing that under these assumptions we can arrange the systems constituting the QCA on the Cayley graph of a group.

We studied the case where such group can be quasi-isometrically embedded in the Euclidean spaces $\mathbb{R}^d$, with $d = 1,2,3$, showing that the minimal nontrivial QCAs are then essentially unique and provide Weyl's equation in the relativistic limit of small wave vectors compared to the inverse of the lattice step, which is taken of the order of Planck's length.

We also showed the unique way in which two Weyl automata can be locally coupled, leading to the Dirac QCA. This QCA provides Dirac's equation in the relativistic limit. We studied first-order corrections to Dirac's evolution due to the discreteness of the QCA lattice. The correction terms lead to a diffusive Schrödinger equation, which expresses the dynamics of the QCA at all scales, in the approximation of narrowband wave packets.

In conclusion, we remark that Lorentz covariance is obeyed only in the relativistic limit $|\mathbf{k}| \ll 1$, whereas the general covariance (corresponding to invariance of $\omega^{E\pm}_{\mathbf{k}}$) is a nonlinear representation of the Lorentz group, with additional invariants in the form of energy and distance scales [31], as in the doubly special relativity [23,24] and in the deformed Lorentz symmetry [25,26], for which the automaton then represents a concrete microscopic theory. Correspondingly, also CPT symmetry of Dirac's QCA is broken at the ultrarelativistic scale.

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APPENDIX A: DERIVATION OF THE WEYL AUTOMATA ON THE BCC LATTICE

In this Appendix we study the unitarity conditions of Eq. (6) on Cayley graphs of $\mathbb{Z}^3$ for $s = 2$. We find two solutions for the bcc lattice, and we prove the impossibility of a unitary solution on the PC and on the rhombohedral lattices.

Before starting the analysis of unitarity conditions on different lattices, let us introduce some notation that will be useful in the following. First of all, let us introduce the polar decomposition of operators $A_{\mathbf{h}}$ as

$$A_{\mathbf{h}} = V_{\mathbf{h}}|A_{\mathbf{h}}|, \tag{A1}$$

with $V_{\mathbf{h}}$ unitary. Notice that, for Bravais lattices, the condition of Eq. (17) with $\mathbf{h}'' = 2\mathbf{h}$ is equivalent to

$$\mathbf{h}'' = \pm 2\mathbf{h}_i, \tag{A2}$$

equivalent to $|A_{\mathbf{h}}||A_{-\mathbf{h}}| = 0$. Now, since $s = 2$ and by definition the $|A_{\pm\mathbf{h}}|$'s are non-null, this can be satisfied only with

$$A_{\mathbf{h}} = \alpha_{\mathbf{h}} V_{\mathbf{h}}|\eta_{\mathbf{h}}\rangle\langle\eta_{\mathbf{h}}|, \quad \alpha_{-\mathbf{h}}A_{-\mathbf{h}} = V_{\mathbf{h}}|\eta_{-\mathbf{h}}\rangle\langle\eta_{-\mathbf{h}}|, \tag{A3}$$

where $\langle\eta_{+\mathbf{h}}|\eta_{-\mathbf{h}}\rangle = 0$, and we can always choose $\alpha_{\mathbf{h}} > 0$ for every $\mathbf{h}$.

1. The bcc case

In the following we take $A_e = 0$ and *a posteriori* we check that there is no other possibility.

Let us now focus on the unitarity conditions. Here, besides $\mathbf{h}'' = \pm 2\mathbf{h}_i$ we have two kinds of conditions. (i) $\mathbf{h}'' = \mathbf{h}_i - \mathbf{h}_j$: In this case there are only two terms in the sums in Eq. (17), thus leading to the same conditions as in Eqs. (A91) and (A93), namely,

$$A^\dagger_{\mathbf{h}_i}A_{\mathbf{h}_j} + A^\dagger_{-\mathbf{h}_j}A_{-\mathbf{h}_i} = 0, \tag{A4}$$

$$A_{\mathbf{h}_i}A^\dagger_{\mathbf{h}_j} + A_{-\mathbf{h}_j}A^\dagger_{-\mathbf{h}_i} = 0. \tag{A5}$$

(ii) $\mathbf{h}'' = \mathbf{h}_i + \mathbf{h}_j$: In this case, the identity $\mathbf{h}_i + \mathbf{h}_j + \mathbf{h}_l + \mathbf{h}_m = 0$ ($ijlm$ a permutation of 1234) implies $\mathbf{h}'' = -\mathbf{h}_l - \mathbf{h}_m$. Consequently, there are four terms in the sums in Eq. (17), leading to the following new conditions:

$$A^\dagger_{\mathbf{h}_i}A_{-\mathbf{h}_j} + A^\dagger_{\mathbf{h}_j}A_{-\mathbf{h}_i} + A^\dagger_{-\mathbf{h}_l}A_{\mathbf{h}_m} + A^\dagger_{-\mathbf{h}_m}A_{\mathbf{h}_l} = 0, \tag{A6}$$

$$A_{\mathbf{h}_j}A^\dagger_{-\mathbf{h}_i} + A_{\mathbf{h}_i}A^\dagger_{-\mathbf{h}_j} + A_{-\mathbf{h}_m}A^\dagger_{\mathbf{h}_l} + A_{-\mathbf{h}_l}A^\dagger_{\mathbf{h}_m} = 0. \tag{A7}$$

Consider now the condition in Eq. (A5). Multiplying on the left by $A^\dagger_{\mathbf{h}_i}$ and on the right by $A_{\mathbf{h}_j}$ we obtain

$$A^\dagger_{\mathbf{h}_i}A_{\mathbf{h}_j}A^\dagger_{\mathbf{h}_i}A_{\mathbf{h}_j} + A^\dagger_{\mathbf{h}_i}A_{-\mathbf{h}_i}A^\dagger_{-\mathbf{h}_j}A_{\mathbf{h}_j} = 0, \tag{A8}$$

and using the condition in Eq. (A2) we have

$$A^\dagger_{\mathbf{h}_i}A_{\mathbf{h}_j}A^\dagger_{\mathbf{h}_i}A_{\mathbf{h}_j} = 0. \tag{A9}$$

Since the transition matrices $A_{\mathbf{h}_i}$ are rank 1, the latter condition can be fulfilled only in the following two cases.

(1) $A_{\mathbf{h}_j}A^\dagger_{\mathbf{h}_i} = 0$. In this case one has clearly $|A_{\mathbf{h}_i}||A_{\mathbf{h}_j}| = |A_{\mathbf{h}_j}||A_{\mathbf{h}_i}| = 0$. In turn, this implies that $\langle\eta_{\mathbf{h}_i}|\eta_{\mathbf{h}_j}\rangle = 0$, i.e., $|\eta_{\mathbf{h}_j}\rangle\langle\eta_{\mathbf{h}_j}| = |\eta_{-\mathbf{h}_i}\rangle\langle\eta_{-\mathbf{h}_i}|$ and

$$\begin{aligned} A_{\mathbf{h}_i} &= \alpha_{\mathbf{h}_i}V_i|\eta_{\mathbf{h}_i}\rangle\langle\eta_{\mathbf{h}_i}|, \quad A_{-\mathbf{h}_i} = \alpha_{-\mathbf{h}_i}V_i|\eta_{-\mathbf{h}_i}\rangle\langle\eta_{-\mathbf{h}_i}|,\\ A_{\mathbf{h}_j} &= \alpha_{\mathbf{h}_j}V_j|\eta_{-\mathbf{h}_i}\rangle\langle\eta_{-\mathbf{h}_i}|, \quad A_{-\mathbf{h}_j} = \alpha_{-\mathbf{h}_j}V_j|\eta_{\mathbf{h}_i}\rangle\langle\eta_{\mathbf{h}_i}|, \end{aligned} \tag{A10}$$

where V_i is a shorthand for $V_{\mathbf{h}_i}$.

(2) $A^\dagger_{\mathbf{h}_i} A_{\mathbf{h}_j} = 0$. In this case, a similar analysis provides the following identities:

$$\begin{aligned} A^\dagger_{\mathbf{h}_i} &= \alpha_{\mathbf{h}_i} V_i |\theta_{\mathbf{h}_i}\rangle\langle\theta_{\mathbf{h}_i}|, \quad A^\dagger_{-\mathbf{h}_i} = \alpha_{-\mathbf{h}_i} V_i |\theta_{-\mathbf{h}_i}\rangle\langle\theta_{-\mathbf{h}_i}|, \\ A^\dagger_{\mathbf{h}_j} &= \alpha_{\mathbf{h}_j} V_j |\theta_{-\mathbf{h}_i}\rangle\langle\theta_{-\mathbf{h}_i}|, \quad A^\dagger_{-\mathbf{h}_j} = \alpha_{-\mathbf{h}_j} V_j |\theta_{\mathbf{h}_i}\rangle\langle\theta_{\mathbf{h}_i}|. \end{aligned} \tag{A11}$$

Now, if $A_{\mathbf{h}_j} A^\dagger_{\mathbf{h}_i} = A_{\mathbf{h}_l} A^\dagger_{\mathbf{h}_i} = 0$—i.e., for both (i,j) and (i,l) condition (1) is satisfied—then by by Eq. (A10) we have

$$A_{\mathbf{h}_j} A^\dagger_{\mathbf{h}_l} = \alpha_{\mathbf{h}_j}\alpha_{\mathbf{h}_l} V_j |\eta_{-\mathbf{h}_i}\rangle\langle\eta_{-\mathbf{h}_i}| V_l^\dagger, \tag{A12}$$

which cannot be null. Similarly, if $A^\dagger_{\mathbf{h}_i} A_{\mathbf{h}_j} = A^\dagger_{\mathbf{h}_i} A_{\mathbf{h}_l} = 0$—i.e., for both (i,j) and (i,l) condition (1) is satisfied—then by Eq. (A11) we have

$$A^\dagger_{\mathbf{h}_j} A_{\mathbf{h}_l} = \alpha_{\mathbf{h}_j}\alpha_{\mathbf{h}_l} V_j |\theta_{-\mathbf{h}_i}\rangle\langle\theta_{-\mathbf{h}_i}| V_l^\dagger, \tag{A13}$$

which cannot be null. Finally, this implies that the conditions of item 1 or item 1 can be satisfied only with one or two different values of j for the same fixed value of i.

Modulo relabelings of the vertices, we then have without loss of generality one of three sets of conditions,

$$\begin{aligned} A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_2} &= A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_3} = A_{\mathbf{h}_2} A^\dagger_{\mathbf{h}_4} = 0, \\ A^\dagger_{\mathbf{h}_2} A_{\mathbf{h}_3} &= A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_4} = A^\dagger_{\mathbf{h}_3} A_{\mathbf{h}_4} = 0, \end{aligned} \tag{A14}$$

or

$$\begin{aligned} A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_2} &= A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_3} = A_{\mathbf{h}_2} A^\dagger_{\mathbf{h}_4} = A_{\mathbf{h}_3} A^\dagger_{\mathbf{h}_4} = 0, \\ A^\dagger_{\mathbf{h}_2} A_{\mathbf{h}_3} &= A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_4} = 0, \end{aligned} \tag{A15}$$

or

$$\begin{aligned} A_{\mathbf{h}_2} A^\dagger_{\mathbf{h}_3} &= A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_4} = 0, \\ A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_2} &= A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_3} = A^\dagger_{\mathbf{h}_2} A_{\mathbf{h}_4} = A^\dagger_{\mathbf{h}_3} A_{\mathbf{h}_4} = 0. \end{aligned} \tag{A16}$$

The conditions in Eqs. (A15) and (A16) lead to the same solutions modulo the exchange of $A_{\mathbf{h}_i}$ and $A^\dagger_{\mathbf{h}_i}$, or equivalently modulo the PT symmetry $\tilde{A}_{\mathbf{k}} \mapsto \tilde{A}^\dagger_{-\mathbf{k}}$. It is then sufficient to solve Eqs. (A14) and (A15).

The number of couples (i,j) for which both conditions (1) and (2) are simultaneously satisfied is limited. Indeed, suppose, e.g., that both $A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_3} = 0$ and $A^\dagger_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_3} = 0$. Then clearly either $A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_2} \neq 0$ or $A^\dagger_{\mathbf{h}_2} A_{\mathbf{h}_1} \neq 0$, otherwise for the couple (2,3) neither condition (1) nor (2) can be satisfied. For a similar reason, either $A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_4} \neq 0$ or $A^\dagger_{\mathbf{h}_4} A_{\mathbf{h}_1} \neq 0$. The same argument can be applied to the couples (2,3) and (3,4). Then the only remaining couple for which both conditions can be simultaneously satisfied is (2,4). Actually, one can prove that in this case, after a little algebra, one can prove that both conditions are satisfied for the couple (2,4).

A necessary condition for isotropy is that

$$\alpha_{\mathbf{h}_i} = \alpha_{\mathbf{h}_j} =: \alpha_+, \quad \alpha_{-\mathbf{h}_i} = \alpha_{-\mathbf{h}_j} =: \alpha_-. \tag{A17}$$

Moreover, considering one couple (i,j) such that either $A^\dagger_{\mathbf{h}_j} A_{\mathbf{h}_i} \neq 0$ or $A_{\mathbf{h}_i} A^\dagger_{\mathbf{h}_j} \neq 0$, by condition (A4) or by condition (A5), respectively, one has

$$\begin{aligned} &\alpha_+^2 |\eta_{-\mathbf{h}_i}\rangle\langle\eta_{-\mathbf{h}_i}| V_j^\dagger V_i |\eta_{\mathbf{h}_i}\rangle\langle\eta_{\mathbf{h}_i}| \\ &\quad + \alpha_-^2 |\eta_{-\mathbf{h}_i}\rangle\langle -\eta_{\mathbf{h}_i}| V_i^\dagger V_j |\eta_{\mathbf{h}_i}\rangle\langle\eta_{\mathbf{h}_i}| = 0, \end{aligned} \tag{A18}$$

which implies $\alpha_+^2 = \alpha_-^2$. Finally, since $\alpha_\pm > 0$ one has $\alpha_+ = \alpha_- =: \alpha$.

Let us first consider the five conditions that are common to both Eqs. (A14) and (A15), namely,

$$A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_2} = A_{\mathbf{h}_1} A^\dagger_{\mathbf{h}_3} = A_{\mathbf{h}_2} A^\dagger_{\mathbf{h}_4} = 0, \tag{A19}$$

$$A^\dagger_{\mathbf{h}_2} A_{\mathbf{h}_3} = A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_4} = 0. \tag{A20}$$

According to Eqs. (A10), the conditions in Eq. (A19) then imply

$$\begin{aligned} A_{\mathbf{h}_1} &= \alpha V_1 M, \quad A_{-\mathbf{h}_1} = \alpha V_1 (I - M), \\ A_{\mathbf{h}_2} &= \alpha V_2 (I - M), \quad A_{-\mathbf{h}_2} = \alpha V_2 M, \\ A_{\mathbf{h}_3} &= \alpha V_3 (I - M), \quad A_{-\mathbf{h}_3} = \alpha V_3 M, \\ A_{\mathbf{h}_4} &= \alpha V_4 M, \quad A_{-\mathbf{h}_4} = \alpha V_4 (I - M), \end{aligned} \tag{A21}$$

where $M := |\eta_{\mathbf{h}_1}\rangle\langle\eta_{\mathbf{h}_1}| = |\eta_{\mathbf{h}_4}\rangle\langle\eta_{\mathbf{h}_4}| = |\eta_{-\mathbf{h}_2}\rangle\langle\eta_{-\mathbf{h}_2}| = |\eta_{-\mathbf{h}_3}\rangle\langle\eta_{-\mathbf{h}_3}|$, with the following constraints on the unitarities V_i,

$$V_2^\dagger V_3 = i\, \mathbf{n}_1 \cdot \boldsymbol{\sigma}, \quad V_4^\dagger V_1 = i\, \mathbf{n}_2 \cdot \boldsymbol{\sigma}, \tag{A22}$$

where $\sigma_z = M - (I - M) = 2M - I$, and the real vectors $\mathbf{n}_i$ lie in the xy plane. Notice that the conditions in Eq. (A20) are now immediately satisfied.

Imposing the conditions in Eq. (A4) and (A5) gives the following new constraints:

$$M V_1^\dagger V_2 (I - M) + M V_2^\dagger V_1 (I - M) = 0, \tag{A23}$$

$$M V_1^\dagger V_3 (I - M) + M V_3^\dagger V_1 (I - M) = 0, \tag{A24}$$

$$V_1 M V_4^\dagger + V_4 (I - M) V_1^\dagger = 0, \tag{A25}$$

$$V_2 (I - M) V_3^\dagger + V_3 M V_2^\dagger = 0, \tag{A26}$$

$$(I - M) V_2^\dagger V_4 M + (I - M) V_4^\dagger V_2 M = 0, \tag{A27}$$

$$(I - M) V_3^\dagger V_4 M + (I - M) V_4^\dagger V_3 M = 0. \tag{A28}$$

While the two conditions of Eq. (A25) and (A26) are easily verified, the remaining four are equivalent to the following conditions:

$$\begin{aligned} [M,(V_1^\dagger V_2 + V_2^\dagger V_1)] &= [M,(V_1^\dagger V_3 + V_3^\dagger V_1)] = 0, \\ [M,(V_2^\dagger V_4 + V_4^\dagger V_2)] &= [M,(V_3^\dagger V_4 + V_4^\dagger V_3)] = 0. \end{aligned} \tag{A29}$$

We can satisfy the first condition in Eq. (A29) in two ways: Either $V_1^\dagger V_2 = \nu(cI + is\sigma_z)$ with $|\nu| = 1$ or $V_1^\dagger V_2 + V_2^\dagger V_1 = \kappa I$ with $|\kappa| = 1$.

In the first case, since $V_1^\dagger V_3 = V_1^\dagger V_2 V_2^\dagger V_3$, we have

$$V_1^\dagger V_3 = i\, \nu \mathbf{n}_3 \cdot \boldsymbol{\sigma}, \tag{A30}$$

where $\mathbf{n}_3 := (c\mathbf{n}_1 - s\mathbf{e}_3 \times \mathbf{n}_1)$. Clearly, $\mathbf{n}_3$ lies in the xy plane. In order to satisfy the conditions in Eq. (A29), ν must then be real, namely $\nu = \pm 1$. Including ν in c,s, we then have

$$V_1^\dagger V_2 = (cI + is\sigma_z), \quad V_1^\dagger V_3 = i\,\mathbf{n}_3 \cdot \boldsymbol{\sigma}, \quad V_1^\dagger V_4 = -i\,\mathbf{n}_2 \cdot \boldsymbol{\sigma}. \tag{A31}$$

In this case, the matrix $\tilde{A}_\mathbf{k}$ has the form

$$\tilde{A}_\mathbf{k} = \alpha V_1 \begin{pmatrix} e^{ik_1} + \omega e^{-ik_2} & i(e^{ik_3} - \theta^* e^{-ik_4}) \\ i(e^{-ik_3} - \theta e^{ik_4}) & e^{-ik_1} + \omega^* e^{ik_2} \end{pmatrix}, \tag{A32}$$

where now $\omega = c + is$, and we choose $\mathbf{n}_3 = (1,0,0)$, while $\theta = (\mathbf{n}_2)_1 + i(\mathbf{n}_2)_2$. The unitarity condition for $\tilde{A}_\mathbf{k}$ finally gives the constraint

$$\alpha^2 \begin{pmatrix} e^{ik_1} + \omega e^{-ik_2} & i(e^{ik_3} - \theta^* e^{-ik_4}) \\ i(e^{-ik_3} - \theta e^{ik_4}) & e^{-ik_1} + \omega^* e^{ik_2} \end{pmatrix} \times \begin{pmatrix} e^{-ik_1} + \omega^* e^{ik_2} & -i(e^{ik_3} - \theta^* e^{-ik_4}) \\ -i(e^{-ik_3} - \theta e^{ik_4}) & e^{ik_1} + \omega e^{-ik_2} \end{pmatrix} = I, \tag{A33}$$

namely,

$$\alpha^2[4 + (\omega - \theta)e^{-i(k_1+k_2)} + (\omega^* - \theta^*)e^{i(k_1+k_2)}] = 1, \tag{A34}$$

for every choice of k_1, k_2 [we remind the reader that $k_1 + k_2 + k_3 + k_4 = 0$, and then $k_3 + k_4 = -(k_1 + k_2)$]. Finally, this implies that $\theta = \omega$ and $\alpha = 1/2$. In order to have $\tilde{A}_{\mathbf{k}=0} = I$ [Eq. (19)], the only possibility is to have $V_1 = X^{-1}$, with

$$X = \frac{1}{2}\begin{pmatrix} 1+\omega & i(1-\omega^*) \\ i(1-\omega) & 1+\omega^* \end{pmatrix}. \tag{A35}$$

Then we have

$$\begin{aligned} \tilde{A}_\mathbf{k} &= \frac{1}{4}\begin{pmatrix} z(\mathbf{k}) & -iw(\mathbf{k})^* \\ -iw(\mathbf{k}) & z(\mathbf{k})^* \end{pmatrix}, \\ z(\mathbf{k}) &:= \zeta^* e^{ik_1} + \zeta e^{-ik_2} + \eta^* e^{-ik_3} + \eta e^{ik_4}, \\ w(\mathbf{k}) &:= \eta e^{ik_1} + \omega\eta e^{-ik_2} - \zeta e^{-ik_3} + \omega\zeta e^{ik_4}, \\ \zeta &= \frac{1+\omega}{4}, \quad \eta = \frac{1-\omega}{4}. \end{aligned} \tag{A36}$$

One can check that the remaining conditions of Eqs. (A6) and (A7) are verified *a posteriori*, since $\tilde{A}_\mathbf{k}$ is unitary.

In the second case we instead impose $V_1^\dagger V_2 + V_2^\dagger V_1 = \kappa I$ without $[V_1^\dagger V_2, M] = 0$, and we have the situation

$$V_1^\dagger V_2 = \nu(cI + is\mathbf{n}_3 \cdot \boldsymbol{\sigma}), \quad V_1^\dagger V_3 = \nu(c'I + is'\mathbf{n}_4 \cdot \boldsymbol{\sigma}), \tag{A37}$$

where

$$c' = -s(\mathbf{n}_1 \cdot \mathbf{n}_3), \quad s'\mathbf{n}_4 = c\mathbf{n}_1 - s(\mathbf{n}_3 \times \mathbf{n}_1). \tag{A38}$$

Now either $\nu = \nu^*$ or $s = s' = 0$. However, if $s = 0$, then $s' = 1$. The only possibility is then $\nu = \nu^* = \pm 1$. Including ν in the coefficients c,c',s,s'. We can also calculate $V_2^\dagger V_4$ and $V_1^\dagger V_4$, obtaining

$$V_1^\dagger V_2 = cI + is\mathbf{n}_3 \cdot \boldsymbol{\sigma}, \tag{A39}$$

$$V_1^\dagger V_3 = c'I + is'\mathbf{n}_4 \cdot \boldsymbol{\sigma}, \tag{A40}$$

$$V_1^\dagger V_4 = -i\mathbf{n}_2 \cdot \boldsymbol{\sigma}, \tag{A41}$$

$$V_2^\dagger V_3 = i\mathbf{n}_1 \cdot \boldsymbol{\sigma}, \tag{A42}$$

$$V_2^\dagger V_4 = -s(\mathbf{n}_2 \cdot \mathbf{n}_3)I - i(c\mathbf{n}_2 + s\mathbf{n}_3 \times \mathbf{n}_2) \cdot \boldsymbol{\sigma}, \tag{A43}$$

$$V_3^\dagger V_4 = -s'(\mathbf{n}_2 \cdot \mathbf{n}_4)I - i(c'\mathbf{n}_2 + s'\mathbf{n}_4 \times \mathbf{n}_2) \cdot \boldsymbol{\sigma}. \tag{A44}$$

One can easily verify that the conditions in Eq. (A29) are all satisfied without further constraints.

Reminding the reader now of the expressions in Eq. (A21), we can impose the conditions in Eqs. (A6) and (A7) as follows:

$$V_1 M V_2^\dagger + V_2(I - M)V_1^\dagger + V_3 M V_4^\dagger + V_4(I - M)V_3^\dagger = 0, \tag{A45}$$

$$V_1 M V_3^\dagger + V_3(I - M)V_1^\dagger + V_2 M V_4^\dagger + V_4(I - M)V_2^\dagger = 0, \tag{A46}$$

$$\begin{aligned} &MV_1^\dagger V_2 M + (I - M)V_2^\dagger V_1(I - M) \\ &\quad + MV_3^\dagger V_4 M + (I - M)V_4^\dagger V_3(I - M) = 0, \end{aligned} \tag{A47}$$

$$\begin{aligned} &MV_1^\dagger V_3 M + (I - M)V_3^\dagger V_1(I - M) \\ &\quad + MV_2^\dagger V_4 M + (I - M)V_4^\dagger V_2(I - M) = 0, \end{aligned} \tag{A48}$$

$$\begin{aligned} &MV_1^\dagger V_4(I - M) + MV_4^\dagger V_1(I - M) \\ &\quad + MV_2^\dagger V_3(I - M) + MV_3^\dagger V_2(I - M) = 0. \end{aligned} \tag{A49}$$

We omit the sixth condition, which is trivially satisfied. The last condition in Eq. (A49) is easily verified using the form of $V_1^\dagger V_4$ and $V_2^\dagger V_3$. Let us now focus on the third and fourth conditions. Substituting the explicit expression for $V_1^\dagger V_2$ and $V_3^\dagger V_4$ in Eq. (A47) and $V_1^\dagger V_3$ and $V_2^\dagger V_4$ in Eq. (A48), and considering that $M = 1/2(I + \sigma_z)$, we obtain

$$\begin{aligned} &cI + is\{\sigma_z, \mathbf{n}_3 \cdot \boldsymbol{\sigma}\} - s'(\mathbf{n}_2 \cdot \mathbf{n}_4)I \\ &\quad - i\{\sigma_z, c'\mathbf{n}_2 - s'\mathbf{n}_2 \times \mathbf{n}_4 \cdot \boldsymbol{\sigma}\} = 0, \\ &c'I + is'\{\sigma_z, \mathbf{n}_4 \cdot \boldsymbol{\sigma}\} - s(\mathbf{n}_2 \cdot \mathbf{n}_3)I \\ &\quad - i\{\sigma_z, c\mathbf{n}_2 - s\mathbf{n}_2 \times \mathbf{n}_3 \cdot \boldsymbol{\sigma}\} = 0, \end{aligned}$$

namely,

$$\begin{aligned} &cI - s'(\mathbf{n}_2 \cdot \mathbf{n}_4)I = 0, \quad s\mathbf{n}_3 \cdot \mathbf{h} + s'\mathbf{n}_2 \times \mathbf{n}_4 \cdot \mathbf{h} = 0, \\ &c'I - s(\mathbf{n}_2 \cdot \mathbf{n}_3)I = 0, \quad s'\mathbf{n}_4 \cdot \mathbf{h} + s\mathbf{n}_2 \times \mathbf{n}_3 \cdot \mathbf{h} = 0. \end{aligned} \tag{A50}$$

Substituting the expression for $s'\mathbf{n}_4$ we have

$$c - c(\mathbf{n}_1 \cdot \mathbf{n}_2) + s\mathbf{n}_1 \cdot (\mathbf{n}_2 \times \mathbf{n}_3) = 0, \tag{A51}$$

$$s\mathbf{n}_3 \cdot \mathbf{h} - c\mathbf{n}_1 \times \mathbf{n}_2 \cdot \mathbf{h} - s(\mathbf{n}_1 \cdot \mathbf{n}_2)\mathbf{n}_3 \cdot \mathbf{h} = 0, \tag{A52}$$

$$c' - s(\mathbf{n}_2 \cdot \mathbf{n}_3) = 0, \tag{A53}$$

$$s\mathbf{n}_1 \times \mathbf{n}_3 \cdot \mathbf{h} + s\mathbf{n}_2 \times \mathbf{n}_3 \cdot \mathbf{h} = 0. \tag{A54}$$

From Eqs. (A38), (A53), and (A54) we immediately conclude

$$s(\mathbf{n}_1 \cdot \mathbf{n}_3) = -s(\mathbf{n}_2 \cdot \mathbf{n}_3), \quad s\mathbf{n}_3 \times \mathbf{h} \cdot \mathbf{n}_1 = -s\mathbf{n}_3 \times \mathbf{h} \cdot \mathbf{n}_2. \tag{A55}$$

For $s = 0$ we recover a special case of the solution as in Eq. (A36). We then consider the case $s \neq 0$. Reminding the reader that we are assuming here $\mathbf{n}_3$ not parallel to $\mathbf{h}$, we have $\mathbf{n}_1 = -\mathbf{n}_2$. Finally, from Eq. (A51) we then conclude that $c = 0$ and $s = \pm 1$. Including s in the definition of $\mathbf{n}_3$, we have

$$V_1^\dagger V_2 = i\mathbf{n}_3\cdot\boldsymbol{\sigma}, \tag{A56}$$

$$V_1^\dagger V_3 = -(\mathbf{n}_1\cdot\mathbf{n}_3)I + i\mathbf{n}_1\times\mathbf{n}_3\cdot\boldsymbol{\sigma}, \tag{A57}$$

$$V_1^\dagger V_4 = i\mathbf{n}_1\cdot\boldsymbol{\sigma}, \tag{A58}$$

$$V_2^\dagger V_3 = i\mathbf{n}_1\cdot\boldsymbol{\sigma}, \tag{A59}$$

$$V_2^\dagger V_4 = (\mathbf{n}_1\cdot\mathbf{n}_3)I - i\mathbf{n}_1\times\mathbf{n}_3\cdot\boldsymbol{\sigma}, \tag{A60}$$

$$V_3^\dagger V_4 = -i[2(\mathbf{n}_1\cdot\mathbf{n}_3)\mathbf{n}_1 - \mathbf{n}_3]\cdot\boldsymbol{\sigma}. \tag{A61}$$

Considering now the condition in Eq. (A45), and multiplying on the left by $V_1^\dagger$ and on the right by V_2, we obtain

$$\begin{aligned} &M + V_1^\dagger V_2(I-M)V_1^\dagger V_2\\ &\quad + V_1^\dagger V_3 M V_4^\dagger V_2 + V_1^\dagger V_4(I-M)V_3^\dagger V_2 = 0. \end{aligned} \tag{A62}$$

Since $V_1^\dagger V_2 = -V_2^\dagger V_1$, $V_2^\dagger V_4 = -V_1^\dagger V_3$, and $V_2^\dagger V_3 = V_1^\dagger V_4$, we obtain

$$2M - (I-\tilde M) - \bar M = 0, \tag{A63}$$

where $\tilde M := V_1^\dagger V_2 M V_2^\dagger V_1$ and $\bar M = V_1^\dagger V_3 M V_3^\dagger V_1$. Finally, this implies $I-\tilde M = \bar M = M$. This implies that $\mathbf{n}_3\cdot\mathbf{h}=0$; namely, also $\mathbf{n}_3$ lies in the xy plane. As a result, we have

$$\tilde A_{\mathbf{k}} = \alpha V_1\begin{pmatrix} e^{ik_1}+\omega e^{-ik_3} & i(e^{ik_2}+\theta e^{-ik_4})\\ i(e^{-ik_2}+\theta^* e^{ik_4}) & e^{-ik_1}+\omega^* e^{ik_3}\end{pmatrix}. \tag{A64}$$

Repeating the same arguments as for Eq. (A36), we get

$$\begin{aligned} \tilde A_{\mathbf{k}} &= \frac14\begin{pmatrix} z'(\mathbf{k}) & -iw'(\mathbf{k})^*\\ -iw'(\mathbf{k}) & z'(\mathbf{k})^*\end{pmatrix},\\ z'(\mathbf{k}) &:= \zeta^* e^{ik_1} + \zeta e^{-ik_3} + \eta^* e^{-ik_2} + \eta e^{ik_4},\\ w'(\mathbf{k}) &:= \eta e^{ik_1} + \omega\eta e^{-ik_3} - \zeta e^{-ik_2} + \omega\zeta e^{ik_4},\\ \zeta &:= \frac{1+\omega}{4},\quad \eta := \frac{1-\omega}{4}. \end{aligned} \tag{A65}$$

We now carry out the analysis for the automaton in Eq. (A36), since the case of Eq. (A65) can be obtained from it by simply exchanging k_2 and k_3.

In the general case of arbitrary ω, we have

$$\begin{aligned} A_{\mathbf{h}_1} &= \begin{pmatrix}\zeta^* & 0\\ -i\eta & 0\end{pmatrix}, & A_{-\mathbf{h}_1} &= \begin{pmatrix}0 & -i\eta^*\\ 0 & \zeta\end{pmatrix},\\ A_{\mathbf{h}_2} &= \begin{pmatrix}0 & i\zeta^*\\ 0 & \eta\end{pmatrix}, & A_{-\mathbf{h}_2} &= \begin{pmatrix}\eta^* & 0\\ i\zeta & 0\end{pmatrix},\\ A_{\mathbf{h}_3} &= \begin{pmatrix}0 & -i\omega^*\eta^*\\ 0 & \zeta^*\end{pmatrix}, & A_{-\mathbf{h}_3} &= \begin{pmatrix}\zeta & 0\\ -i\omega\eta & 0\end{pmatrix},\\ A_{\mathbf{h}_4} &= \begin{pmatrix}\eta & 0\\ -i\omega\zeta & 0\end{pmatrix}, & A_{-\mathbf{h}_4} &= \begin{pmatrix}0 & -i\omega^*\zeta^*\\ 0 & \eta^*\end{pmatrix}, \end{aligned} \tag{A66}$$

with $\zeta = (1+\omega)/4$ and $\eta = (1-\omega)/4$.

The unitary $A_{\mathbf{k}}$ can be rewritten as

$$A_{\mathbf{k}} = \sum_{j=1}^{4}(-iA_j\sin k_j + B_j\cos k_j), \tag{A67}$$

with

$$A_i = A_{\mathbf{h}_i} - A_{-\mathbf{h}_i},\quad B_i = A_{\mathbf{h}_i} + A_{-\mathbf{h}_i}. \tag{A68}$$

Considering the expressions in Eq. (A66), we can conclude the following identities:

$$\begin{aligned} B_1 &= A_1\sigma_z, & B_4 &= A_4\sigma_z,\\ B_2 &= -A_2\sigma_z, & B_3 &= -A_3\sigma_z. \end{aligned} \tag{A69}$$

Using now the trigonometric identities

$$\begin{aligned} \sin(\alpha+\beta+\gamma) &= \sin\alpha\cos\beta\cos\gamma + \cos\alpha\sin\beta\cos\gamma\\ &\quad + \cos\alpha\cos\beta\sin\gamma - \sin\alpha\sin\beta\sin\gamma,\\ \cos(\alpha+\beta+\gamma) &= \cos\alpha\cos\beta\cos\gamma - \cos\alpha\sin\beta\sin\gamma\\ &\quad - \sin\alpha\cos\beta\sin\gamma - \sin\alpha\sin\beta\cos\gamma, \end{aligned} \tag{A70}$$

we can rewrite Eq. (A36) as

$$\begin{aligned} \tilde A_{\mathbf{k}} &= -i\alpha_x\, s_xc_yc_z - \beta_x\, c_xs_ys_z - i\alpha_y\, c_xs_yc_z - \beta_y\, s_xc_ys_z\\ &\quad - i\alpha_z\, c_xc_ys_z - \beta_z\, s_xs_yc_z + i\mu\, s_xs_ys_z + I\, c_xc_yc_z, \end{aligned} \tag{A71}$$

where

$$s_\nu := \sin\frac{k_\nu}{\sqrt3},\quad c_\nu := \cos\frac{k_\nu}{\sqrt3},\quad \nu = x,y,z, \tag{A72}$$

and we used the condition $\sum_i B_i = I$, which is a consequence of Eq. (19), and the definitions

$$\begin{aligned} \alpha_x &:= A_1 + A_2 - A_3 - A_4,\\ \alpha_y &:= A_1 - A_2 + A_3 - A_4,\\ \alpha_z &:= A_1 - A_2 - A_3 + A_4,\\ \mu &:= A_1 + A_2 + A_3 + A_4,\\ \beta_x &:= B_1 + B_2 - B_3 - B_4,\\ \beta_y &:= B_1 - B_2 + B_3 - B_4,\\ \beta_z &:= B_1 - B_2 - B_3 + B_4. \end{aligned} \tag{A73}$$

Exploiting Eq. (A69), we obtain

$$\begin{aligned} \beta_x &= (A_1 - A_2 + A_3 - A_4)\sigma_z = \alpha_y\sigma_z,\\ \beta_y &= (A_1 + A_2 - A_3 - A_4)\sigma_z = \alpha_x\sigma_z,\\ \beta_z &= (A_1 + A_2 + A_3 + A_4)\sigma_z = \mu\sigma_z. \end{aligned} \tag{A74}$$

By direct calculation we can get

$$\begin{aligned} \alpha_x &= \begin{pmatrix} \zeta^*-\eta^*+\zeta-\eta & i(\eta^*+\zeta^*+\omega^*\eta^*-\omega^*\zeta^*)\\ -i(\eta+\zeta+\omega\eta-\omega\zeta) & -\zeta+\eta-\zeta^*+\eta^*\end{pmatrix}\\ &= \begin{pmatrix} \mathrm{Re}\,\omega & \frac{i}{2}(1-\omega^{*2})\\ -\frac{i}{2}(1-\omega^2) & -\mathrm{Re}\,\omega\end{pmatrix},\\ \alpha_y &= \begin{pmatrix} \zeta^*+\eta^*-\zeta-\eta & i(\eta^*-\zeta^*-\omega^*\eta^*-\omega^*\zeta^*)\\ -i(\eta-\zeta-\omega\eta-\omega\zeta) & -\zeta-\eta+\zeta^*+\eta^*\end{pmatrix}\\ &= \begin{pmatrix} 0 & -i\omega^*\\ i\omega & 0\end{pmatrix}, \end{aligned}$$

$$\begin{aligned}\alpha_z &= \begin{pmatrix} \zeta^*+\eta^*+\zeta+\eta & i(\eta^*-\zeta^*+\omega^*\eta^*+\omega^*\zeta^*) \\ -i(\eta-\zeta+\omega\eta+\omega\zeta) & -\zeta-\eta-\zeta^*-\eta^* \end{pmatrix} \\ &= \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \\ \mu &= \begin{pmatrix} \zeta^*-\eta^*-\zeta+\eta & i(\eta^*+\zeta^*-\omega^*\eta^*+\omega^*\zeta^*) \\ -i(\eta+\zeta-\omega\eta+\omega\zeta) & -\zeta+\eta+\zeta^*-\eta^* \end{pmatrix} \\ &= \begin{pmatrix} -i\,\mathrm{Im}\,\omega & \frac{i}{2}(1+\omega^{*2}) \\ -\frac{i}{2}(1+\omega^2) & -i\,\mathrm{Im}\,\omega \end{pmatrix}. \end{aligned} \tag{A75}$$

Let us now consider the point symmetries of the Bravais lattice, namely the symmetries of the cubic cell. There are two groups that are transitive over S_+ and have no trivial transitive subgroups: (1) the group L_3 generated by the rotations around the four ternary axes along the diagonals of the cube; (2) the group L_2 of binary rotations around the three principal axes of the cube. Using the covariance under any of these groups, thus permuting and/or changing the signs of the α matrices, it is easy to see that an identity must hold,

$$2\mathrm{Re}\,\omega I = \{\alpha_x,\alpha_z\} = 0, \tag{A76}$$

namely, $\omega = \pm i$. This condition selects two solutions that can be expressed in terms of the following matrices:

$$\begin{aligned} &\alpha_x^\pm := -\sigma_y, \quad \beta_x^\pm := \pm i\sigma_y, \\ &\alpha_y^\pm := \mp\sigma_x, \quad \beta_y^\pm := -i\sigma_x, \\ &\alpha_z^\pm := \sigma_z, \quad \beta_z^\pm := \mp i\sigma_z, \\ &\mu^\pm := \mp iI. \end{aligned} \tag{A77}$$

By conjugating with $\exp(-i\pi\sigma_z/4)$ (which is a local conjugation on the automaton, changing only the representation), we get the simpler representation

$$\begin{aligned} &\alpha_x^\pm := \sigma_x, \quad \beta_x^\pm := \mp i\sigma_x, \\ &\alpha_y^\pm := \mp\sigma_y, \quad \beta_y^\pm := -i\sigma_y, \\ &\alpha_z^\pm := \sigma_z, \quad \beta_z^\pm := \mp i\sigma_z, \end{aligned} \tag{A78}$$

which satisfies

$$\beta_x^\pm = \mp i\alpha_x^\pm, \quad \beta_y^\pm = \pm i\alpha_y^\pm, \quad \beta_z^\pm = \mp i\alpha_z^\pm. \tag{A79}$$

In this representation, the automata in Eq. (A71) with unitary operator $\tilde{A}_{\mathbf{k}}^\pm$ corresponding to $\omega = \pm i$ become

$$\begin{aligned} \tilde{A}_{\mathbf{k}}^\pm &= \frac{1}{4}\begin{pmatrix} z(\mathbf{k}) & -w(\mathbf{k})^* \\ w(\mathbf{k}) & z(\mathbf{k})^* \end{pmatrix}, \\ z(\mathbf{k}) &:= \zeta^* e^{ik_1} + \zeta e^{-ik_2} + \zeta e^{-ik_3} + \zeta^* e^{ik_4}, \\ w(\mathbf{k}) &:= \zeta^* e^{ik_1} + \zeta e^{-ik_2} - \zeta e^{-ik_3} - \zeta^* e^{ik_4}, \\ \zeta &= \frac{1\pm i}{4}, \end{aligned} \tag{A80}$$

and can be written as

$$\tilde{A}_{\mathbf{k}}^\pm = I d_{\mathbf{k}}^\pm - i\boldsymbol{\alpha}^\pm \cdot \mathbf{a}_{\mathbf{k}}^\pm, \tag{A81}$$

where

$$\begin{aligned} &(a_{\mathbf{k}}^\pm)_x := s_x c_y c_z \mp c_x s_y s_z, \quad (a_{\mathbf{k}}^\pm)_y := c_x s_y c_z \pm s_x c_y s_z, \\ &(a_{\mathbf{k}}^\pm)_z := c_x c_y s_z \mp s_x s_y c_z, \quad d_{\mathbf{k}}^\pm := c_x c_y c_z \pm s_x s_y s_z, \end{aligned} \tag{A82}$$

while $\boldsymbol{\alpha}^\pm$ is the vector of matrices defined in Eq. (A78). The dispersion relation is given by

$$\omega_{\mathbf{k}}^{A^\pm} = \arccos(c_x c_y c_z \pm s_x s_y s_z). \tag{A83}$$

In the new representation, the matrices $A_{\mathbf{h}_i}$ read

$$\begin{aligned} &A_{\mathbf{h}_1} = \begin{pmatrix} \zeta^* & 0 \\ \zeta^* & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \begin{pmatrix} 0 & -\zeta \\ 0 & \zeta \end{pmatrix}, \\ &A_{\mathbf{h}_2} = \begin{pmatrix} 0 & \zeta^* \\ 0 & \zeta^* \end{pmatrix}, \quad A_{-\mathbf{h}_2} = \begin{pmatrix} \zeta & 0 \\ -\zeta & 0 \end{pmatrix}, \\ &A_{\mathbf{h}_3} = \begin{pmatrix} 0 & -\zeta^* \\ 0 & \zeta^* \end{pmatrix}, \quad A_{-\mathbf{h}_3} = \begin{pmatrix} \zeta & 0 \\ \zeta & 0 \end{pmatrix}, \\ &A_{\mathbf{h}_4} = \begin{pmatrix} \zeta^* & 0 \\ -\zeta^* & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_4} = \begin{pmatrix} 0 & \zeta \\ 0 & \zeta \end{pmatrix}. \end{aligned} \tag{A84}$$

As we already noticed, the isotropic automata among the family of Eq. (A65)—more precisely the ones obtained by conjugating with $e^{-i\frac{\pi}{4}\sigma_z}$—can be obtained by those in Eq. (A81) by simply exchanging k_2 and k_3, namely k_x and k_y. We then have

$$\begin{aligned} \tilde{A'}_{\mathbf{k}}^\pm = &-i\alpha_x^\pm(s_y c_x c_z \mp c_y s_x s_z) - i\alpha_y^\pm(c_y s_x c_z \pm s_y c_x s_z) \\ &- i\alpha_z^\pm(c_x c_y s_z \mp s_x s_y c_z) + I(c_x c_y c_z \pm s_x s_y s_z). \end{aligned} \tag{A85}$$

It is more convenient to conjugate the two automata in the last expression in such a way that σ_x is multiplied by the coefficient in the second line and σ_y by that in the first line. This can be achieved, e.g., by conjugating the spatial part of the automaton with the rotation of $-\pi/2$ around the z axis, thus obtaining the two following automata:

$$\begin{aligned} \tilde{Z}_{\mathbf{k}}^\pm = &-i\alpha_x^\pm(s_x c_y c_z \pm c_x s_y s_z) - i\alpha_y^\pm(c_x s_y c_z \mp s_x c_y s_z) \\ &- i\alpha_z^\pm(c_x c_y s_z \pm s_x s_y c_z) + I(c_x c_y c_z \mp s_x s_y s_z). \end{aligned} \tag{A86}$$

These automata, however, are completely equivalent to the ones in Eq. (A81), precisely, $\tilde{A}_{\mathbf{k}}^\pm = \tilde{Z}_{\mathbf{k}}^\mp$.

Using the expressions in Eqs. (A81) and (A86), one can easily verify that the two automata $\tilde{A}_{\mathbf{k}}^\pm$ are covariant under the group L_2 of binary rotations around the coordinate axes. Indeed, each rotation changes the sign of two components k_ν, leaving the third unchanged. The coefficient of I does not change under any of these transformations, while the coefficients of the two Pauli matrices, corresponding to the two directions changing sign, change their sign; the remaining one is unchanged. For example, for the transformation $(x,y,z) \mapsto (-x,-y,z)$ we have

$$s_x c_y c_z \mp c_x s_y s_z \ \mapsto\ -(s_x c_y c_z \mp c_x s_y s_z), \tag{A87}$$

$$c_x s_y c_z \pm s_x c_y s_z \ \mapsto\ -(c_x s_y c_z \pm s_x c_y s_z), \tag{A88}$$

$$c_x c_y s_z \mp s_x s_y c_z \ \mapsto\ (c_x c_y s_z \mp s_x s_y c_z). \tag{A89}$$

These changes of sign can be compensated by conjugating the automaton by $i\sigma_z$, which is the element of $\mathbb{SU}(2)$ representing the same rotation. Being each automaton covariant under the group L'_2 which acts transitively over S_+, we conclude that both automata are isotropic, with $L = L_2$. Notice that none of the automata is covariant under L_3 (one can easily see that the permutation covariance is broken by the difference in the relative sign between the two terms of the x,z components and the y component of $\mathbf{a}^{\pm}_{\mathbf{k}}$). However, this is not required for the automata isotropy.

We can now check that adding equations including the term A_e gives $A_e = 0$. In fact, we must have

$$A_e \tilde{A}^{\pm}_{\mathbf{k}} + \text{H.c.} = 0, \quad \forall\, \mathbf{k} \in B. \tag{A90}$$

However, one can immediately check that $A_e \tilde{A}^{\pm}_{\mathbf{k}}$ cannot be anti-Hermitian for all $\mathbf{k}$, by taking $\mathbf{k} = (0,0,0)$ and $\mathbf{k} = (\pi/2,\pi/2,-\pi/2)$.

2. The PC case

We now show that it is impossible to satisfy the unitarity conditions in Eq. (17) on a PC lattice. The generators $\mathbf{h}$ in this case are six, which can be classified as $S_\pm = \{\pm\mathbf{h}_1, \pm\mathbf{h}_2, \pm\mathbf{h}_3\}$. First, consider the directions $\mathbf{h}'' = \mathbf{h}_i \pm \mathbf{h}_j$. In this case, Eq. (17) provides the following conditions:

$$A^\dagger_{\mathbf{h}_i} A_{\mathbf{h}_j} + A^\dagger_{-\mathbf{h}_j} A_{-\mathbf{h}_i} = 0, \tag{A91}$$

$$A^\dagger_{\mathbf{h}_i} A_{-\mathbf{h}_j} + A^\dagger_{\mathbf{h}_j} A_{-\mathbf{h}_i} = 0, \tag{A92}$$

$$A_{\mathbf{h}_i} A^\dagger_{\mathbf{h}_j} + A_{-\mathbf{h}_j} A^\dagger_{-\mathbf{h}_i} = 0, \tag{A93}$$

$$A_{-\mathbf{h}_i} A^\dagger_{\mathbf{h}_j} + A_{-\mathbf{h}_j} A^\dagger_{\mathbf{h}_i} = 0. \tag{A94}$$

Multiplying the conditions in Eq. (A93) by $A^\dagger_{\mathbf{h}_i}$ on the left and by $A_{\mathbf{h}_j}$ on the right,

$$|A_{\mathbf{h}_i}|^2 |A_{\mathbf{h}_j}|^2 + A^\dagger_{\mathbf{h}_i} A_{-\mathbf{h}_j} A^\dagger_{-\mathbf{h}_i} A_{\mathbf{h}_j} = 0, \tag{A95}$$

and exploiting the conditions in Eqs. (A92) and (A93) and their adjoints, the left-hand side of Eq. (A95) can be rewritten as follows:

$$\left[|A_{\mathbf{h}_i}|^2, |A_{\mathbf{h}_j}|^2\right] = 0. \tag{A96}$$

This implies that the $|A_{\mathbf{h}_i}|$'s are all diagonal in the same basis $\{|\eta_+\rangle, |\eta_-\rangle\}$, and we can write $A_{\mathbf{h}_i}$ in the form

$$A_{\mathbf{h}_i} = \alpha_i V_i |\eta_+\rangle\langle\eta_+|, \quad A_{-\mathbf{h}_i} = \beta_i V_i |\eta_-\rangle\langle\eta_-|, \tag{A97}$$

where $V_i := V_{\mathbf{h}_i}$, and $\alpha_i,\beta_i > 0$. In order to satisfy the conditions in Eq. (A93) and (A94); however, one has to fulfill also the equations

$$\alpha_i\alpha_j V_i |\eta_+\rangle\langle\eta_+| V^\dagger_j + \beta_i\beta_j V_j |\eta_-\rangle\langle\eta_-| V^\dagger_i = 0, \tag{A98}$$

and upon multiplying both sides by $V^\dagger_i$ on the left and by V_j on the right, one has

$$\alpha_i\alpha_j |\eta_+\rangle\langle\eta_+| + \beta_i\beta_j V^\dagger_i V_j |\eta_-\rangle\langle\eta_-| V^\dagger_i V_j = 0, \tag{A99}$$

that implies $V^\dagger_i V_j |\eta_-\rangle \propto |\eta_+\rangle$, namely,

$$V^\dagger_i V_j = \mathbf{n}_{ij} \cdot \boldsymbol{\sigma}, \tag{A100}$$

where σ_k denote the Pauli matrices in the basis η_+,η_-, and where the complex vector $\mathbf{n}_{ij}$ is of the form $\mathbf{n}_{ij} = (a_{ij},b_{ij},0)$. Now, using the identity

$$(\mathbf{a}\cdot\boldsymbol{\sigma})(\mathbf{b}\cdot\boldsymbol{\sigma}) = \mathbf{a}\cdot\mathbf{b}\, I + i(\mathbf{a}\times\mathbf{b})\cdot\boldsymbol{\sigma}, \tag{A101}$$

for consistency, one must have

$$\mathbf{n}_{ij}\cdot\mathbf{n}_{jk} = 0, \quad i\,\mathbf{n}_{ij}\times\mathbf{n}_{jk} = \mathbf{n}_{ik}, \tag{A102}$$

which cannot be satisfied for all vectors $\mathbf{n}_{ij}$ coplanar, namely of the form $\mathbf{n}_{ij} = (a_{ij},b_{ij},0)$. Therefore one cannot fulfill the unitarity requirement for the PC lattice.

3. The rhombohedral case

The rhombohedral lattice corresponds to the presentation of $\mathbb{Z}^3$ involving six vectors constrained by the relators $\mathbf{h}_1 - \mathbf{h}_2 = \mathbf{h}_4$, $\mathbf{h}_2 - \mathbf{h}_3 = \mathbf{h}_5$, and $\mathbf{h}_3 - \mathbf{h}_1 = \mathbf{h}_6$. Since the relators that are useful for the unitarity condition are those of length four, we conveniently change the presentation to the equivalent one:

$$\begin{aligned} &\mathbf{h}_1 - \mathbf{h}_3 = \mathbf{h}_4 + \mathbf{h}_5, \quad \mathbf{h}_2 - \mathbf{h}_1 = \mathbf{h}_5 + \mathbf{h}_6,\\ &\mathbf{h}_3 - \mathbf{h}_2 = \mathbf{h}_6 + \mathbf{h}_4. \end{aligned} \tag{A103}$$

The unitarity conditions then involve the following conditions:

$$\begin{aligned}
&A^\dagger_{\mathbf{h}_1} A_{-\mathbf{h}_2} + A^\dagger_{\mathbf{h}_2} A_{-\mathbf{h}_1} = 0, \quad A^\dagger_{\mathbf{h}_1} A_{-\mathbf{h}_4} + A^\dagger_{\mathbf{h}_4} A_{-\mathbf{h}_1} = 0,\\
&A^\dagger_{\mathbf{h}_2} A_{-\mathbf{h}_3} + A^\dagger_{\mathbf{h}_3} A_{-\mathbf{h}_2} = 0, \quad A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_6} + A^\dagger_{-\mathbf{h}_6} A_{-\mathbf{h}_1} = 0,\\
&A^\dagger_{\mathbf{h}_3} A_{-\mathbf{h}_1} + A^\dagger_{\mathbf{h}_1} A_{-\mathbf{h}_3} = 0, \quad A^\dagger_{\mathbf{h}_2} A_{\mathbf{h}_4} + A^\dagger_{-\mathbf{h}_4} A_{-\mathbf{h}_2} = 0,\\
&A^\dagger_{\mathbf{h}_4} A_{\mathbf{h}_5} + A^\dagger_{-\mathbf{h}_5} A_{-\mathbf{h}_4} = 0, \quad A^\dagger_{\mathbf{h}_2} A_{-\mathbf{h}_5} + A^\dagger_{\mathbf{h}_5} A_{-\mathbf{h}_2} = 0,\\
&A^\dagger_{\mathbf{h}_5} A_{\mathbf{h}_6} + A^\dagger_{-\mathbf{h}_6} A_{-\mathbf{h}_5} = 0, \quad A^\dagger_{\mathbf{h}_3} A_{\mathbf{h}_5} + A^\dagger_{-\mathbf{h}_5} A_{-\mathbf{h}_3} = 0,\\
&A^\dagger_{\mathbf{h}_6} A_{\mathbf{h}_4} + A^\dagger_{-\mathbf{h}_4} A_{-\mathbf{h}_6} = 0, \quad A^\dagger_{\mathbf{h}_3} A_{-\mathbf{h}_6} + A^\dagger_{\mathbf{h}_6} A_{-\mathbf{h}_3} = 0.
\end{aligned} \tag{A104}$$

As in the case of the bcc, for each condition of the kind $A^\dagger_{\mathbf{h}_i} A_{\mathbf{h}_j} + A^\dagger_{-\mathbf{h}_j} A_{-\mathbf{h}_i}$, one has either (a) $A^\dagger_{\mathbf{h}_i} A_{\mathbf{h}_j} = 0$ or (b) $A_{\mathbf{h}_j} A^\dagger_{\mathbf{h}_i} = 0$. However, no more than two couples (i,j) with the same i or j can satisfy the same condition (a) or (b). This implies that all the couples appearing in Eq. (A104) must be partitioned in two subsets corresponding to conditions (a) and (b), consistently with the requirement that no more than two couples with the same $\mathbf{h}_i$ appear in the same set. It turns out that there are only two ways of arranging the couples, and both of them lead to commutation relations of the kind $[|A_{\mathbf{h}_i}|, |A_{\mathbf{h}_j}|] = 0$. Then either $A^\dagger_{\mathbf{h}_i} A_{\mathbf{h}_j} = 0$ or $A^\dagger_{\mathbf{h}_i} A_{-\mathbf{h}_j} = 0$. Now from the relators

$$\begin{aligned} &\mathbf{h}_1 - \mathbf{h}_5 = \mathbf{h}_4 + \mathbf{h}_3, \quad \mathbf{h}_2 - \mathbf{h}_6 = \mathbf{h}_5 + \mathbf{h}_1,\\ &\mathbf{h}_3 - \mathbf{h}_4 = \mathbf{h}_6 + \mathbf{h}_2, \end{aligned} \tag{A105}$$

we can write the following equations involved by the unitarity conditions:

$$\begin{aligned}
&A^\dagger_{\mathbf{h}_1} A_{\mathbf{h}_5} + A^\dagger_{\mathbf{h}_5} A_{\mathbf{h}_1} + A^\dagger_{\mathbf{h}_4} A_{-\mathbf{h}_3} + A^\dagger_{\mathbf{h}_3} A_{-\mathbf{h}_4} = 0,\\
&A^\dagger_{\mathbf{h}_2} A_{\mathbf{h}_6} + A^\dagger_{\mathbf{h}_6} A_{\mathbf{h}_2} + A^\dagger_{\mathbf{h}_5} A_{-\mathbf{h}_1} + A^\dagger_{\mathbf{h}_1} A_{-\mathbf{h}_5} = 0,\\
&A^\dagger_{\mathbf{h}_3} A_{\mathbf{h}_4} + A^\dagger_{\mathbf{h}_4} A_{\mathbf{h}_3} + A^\dagger_{\mathbf{h}_6} A_{-\mathbf{h}_2} + A^\dagger_{\mathbf{h}_2} A_{-\mathbf{h}_6} = 0.
\end{aligned} \tag{A106}$$

If, e.g., $A^\dagger_{\pm\mathbf{h}_1} A_{\pm\mathbf{h}_5} = 0$, then $A^\dagger_{\mp\mathbf{h}_4} A_{\pm\mathbf{h}_3} = 0$, and then $A^\dagger_{\pm\mathbf{h}_3} A_{\pm\mathbf{h}_4} \neq 0$. Continuing with this sequence of implications, one comes to the contradiction that $A^\dagger_{\pm\mathbf{h}_1} A_{\mp\mathbf{h}_5} \neq 0$. A similar contradiction can be derived in the opposite case, where $A^\dagger_{\pm\mathbf{h}_1} A_{\pm\mathbf{h}_5} \neq 0$.

This proves the impossibility of a unitary automaton on the rhombohedral lattice.

APPENDIX B: COUPLING OF WEYL AUTOMATA

In this Appendix we show the unique possible automaton coupling two Weyl automata. The derivation is independent of the dimension and can thus be applied to all the solutions derived in the paper.

Imposing unitarity on the matrix $\tilde{A}'_{\mathbf{k}}$ of Eq. (35), we obtain the equations

$$\begin{aligned} |x|^2 I + y^2 BB^\dagger = I, \quad |x|^2 I + z^2 C^\dagger C = I,\\ z^2 CC^\dagger + |t|^2 I = I, \quad y^2 B^\dagger B + |t|^2 I = I,\\ xz\tilde{A}_{\mathbf{k}} C^\dagger + yt^* B\tilde{D}^\dagger_{\mathbf{k}} = 0, \quad x^* y\tilde{A}^\dagger_{\mathbf{k}} B + ztC^\dagger \tilde{D}_{\mathbf{k}} = 0,\\ zx^* C\tilde{A}^\dagger_{\mathbf{k}} + ty\tilde{D}_{\mathbf{k}} B^\dagger = 0, \quad xyB^\dagger \tilde{A}_{\mathbf{k}} + t^* z\tilde{D}^\dagger_{\mathbf{k}} C = 0, \end{aligned} \tag{B1}$$

which imply

$$\begin{aligned} B^\dagger B = C^\dagger C = I, \quad BB^\dagger = CC^\dagger = I,\\ y^2 = z^2, \quad x\tilde{A}_{\mathbf{k}} = -t^* B\tilde{D}^\dagger_{\mathbf{k}} C, \end{aligned} \tag{B2}$$

$$|x|^2 + y^2 = z^2 + |t|^2 = 1. \tag{B3}$$

Specializing to $\mathbf{k} = 0$ we obtain $\tilde{A}_{\mathbf{k}=0} = \tilde{D}_{\mathbf{k}=0} = I$, and then by Eq. (B2) $C = e^{i\theta} B^\dagger$, where $e^{i\theta} := -e^{i\arg[xt]}$. We can then prove that

$$\tilde{A}'_{\mathbf{k}} := \begin{pmatrix} x\tilde{A}_{\mathbf{k}} & yB \\ ye^{i\theta} B^\dagger & -x^* e^{i\theta} B^\dagger \tilde{A}^\dagger_{\mathbf{k}} B \end{pmatrix}, \tag{B4}$$

and this is equivalent to the automaton

$$\tilde{A}''_{\mathbf{k}} := \begin{pmatrix} x\tilde{A}_{\mathbf{k}} & iyI \\ -iye^{i\theta} I & -x^* e^{i\theta} \tilde{A}^\dagger_{\mathbf{k}} \end{pmatrix}, \tag{B5}$$

through conjugation by

$$\tilde{U} = \begin{pmatrix} I & 0 \\ 0 & iB \end{pmatrix}, \tag{B6}$$

namely, $\tilde{A}''_{\mathbf{k}} = \tilde{U}\tilde{A}'_{\mathbf{k}}\tilde{U}^\dagger$. Diagonalizing the matrix in Eq. (B5), one can prove that it is not restrictive to take $e^{i\theta} = \pm 1$ and $x > 0$ (other choices would simply lead to a different determinant for $\tilde{A}''_{\mathbf{k}}$). Indeed, the choice of sign for $e^{i\theta}$ and of the phase of x affect the spectrum of $\tilde{A}''_{\mathbf{k}}$ only through multiplication of the eigenvalues by a constant phase. Upon choosing $\tilde{A}_{\mathbf{k}}$ as one of the Weyl automata for $d = 1,2,3$, we then obtain the Dirac automata

$$\tilde{E}_{\mathbf{k}} := \begin{pmatrix} n\tilde{A}_{\mathbf{k}} & imI \\ imI & n\tilde{A}^\dagger_{\mathbf{k}} \end{pmatrix}, \tag{B7}$$

with $n,m \geqslant 0$ and $n^2 + m^2 = 1$.

The dispersion relation for these automata is easily calculated by performing the block-diagonal unitary transformation $T_{\mathbf{k}}$ with blocks diagonalizing $\tilde{A}_{\mathbf{k}}$, leading to

$$\tilde{E}''_{\mathbf{k}} = T_{\mathbf{k}}\tilde{E}_{\mathbf{k}}T^\dagger_{\mathbf{k}} = \begin{pmatrix} ne^{-i\omega^A_{\mathbf{k}}} & 0 & im & 0 \\ 0 & ne^{i\omega^A_{\mathbf{k}}} & 0 & im \\ im & 0 & ne^{i\omega^A_{\mathbf{k}}} & 0 \\ 0 & im & 0 & ne^{-i\omega^A_{\mathbf{k}}} \end{pmatrix}, \tag{B8}$$

and then diagonalizing the two 2×2 blocks $\tilde{E}''^{j}_{\mathbf{k}}$, $j = e,o$ corresponding to the even and odd rows and columns, respectively, thus obtaining

$$\omega^E_{\mathbf{k}} := \arccos\left[\sqrt{1-m^2}\cos\omega^A_{\mathbf{k}}\right]. \tag{B9}$$

Notice that for mass $m = 0$ we have $\omega^E_{\mathbf{k}} = \omega^A_{\mathbf{k}}$. The group velocities are

$$\mathbf{v}^E_{\mathbf{k}} = \frac{\sqrt{1-m^2}\sin\omega^A_{\mathbf{k}}}{\sqrt{m^2 + (1-m^2)\sin^2\omega^A_{\mathbf{k}}}}\mathbf{v}^A_{\mathbf{k}}, \tag{B10}$$

where $\mathbf{v}^A_{\mathbf{k}}$ is the group velocity of the corresponding Weyl automaton A.

The projections $\Pi^\pm_{\mathbf{k}}$ on particle and antiparticle states, corresponding to the degenerate eigenspaces of $\tilde{E}_{\mathbf{k}}$, can be calculated as follows. Consider the diagonal expression for the unitary $\tilde{E}''_{\mathbf{k}}$ in Eq. (B8),

$$\begin{aligned} \tilde{E}''_{\mathbf{k}} = {} & (|\psi^+_{\mathbf{k}}\rangle\langle\psi^+_{\mathbf{k}}|_e + |\psi^+_{\mathbf{k}}\rangle\langle\psi^+_{\mathbf{k}}|_o)e^{-i\omega^E_{\mathbf{k}}}\\ & +(|\psi^-_{\mathbf{k}}\rangle\langle\psi^-_{\mathbf{k}}|_e + |\psi^+_{\mathbf{k}}\rangle\langle\psi^+_{\mathbf{k}}|_0)e^{i\omega^E_{\mathbf{k}}}, \end{aligned} \tag{B11}$$

where $|\psi^l_{\mathbf{k}}\rangle\langle\psi^l_{\mathbf{k}}|_j$ is the projection on an eigenvector of $\tilde{E}''_{\mathbf{k}}$, the label j refers to the block to which the eigenvector pertains, and the superscript sign l refers to the eigenvalue. Now since

$$\tilde{E}''^{j}_{\mathbf{k}} = n\cos\omega^A_{\mathbf{k}} I + i\left\{m\sigma_x + s(j)n\sin\omega^A_{\mathbf{k}}\sigma_z\right\}, \tag{B12}$$

with $s(o) = -1$ and $s(e) = 1$, we have

$$\left|\psi^l_{\mathbf{k}}\right\rangle\!\left\langle\psi^l_{\mathbf{k}}\right|_j = \frac{1}{2}\left\{I + l\frac{m\sigma_x + s(j)n\sin\omega^E_{\mathbf{k}}\sigma_z}{\sqrt{1-n^2\cos^2\omega^E_{\mathbf{k}}}}\right\}. \tag{B13}$$

We can thus write an expression for $T_{\mathbf{k}}\Pi^\pm_{\mathbf{k}}T^\dagger_{\mathbf{k}}$

$$T_{\mathbf{k}}\Pi^\pm_{\mathbf{k}}T^\dagger_{\mathbf{k}} = |\psi^\pm_{\mathbf{k}}\rangle\langle\psi^\pm_{\mathbf{k}}|_e + |\psi^\pm_{\mathbf{k}}\rangle\langle\psi^\pm_{\mathbf{k}}|_o, \tag{B14}$$

namely,

$$T_{\mathbf{k}}\Pi^\pm_{\mathbf{k}}T^\dagger_{\mathbf{k}} = \frac{1}{2}\begin{pmatrix} 1 \mp \frac{n\sin\omega^A_{\mathbf{k}}}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} & 0 & \pm\frac{im}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} & 0 \\ 0 & 1 \pm \frac{n\sin\omega^A_{\mathbf{k}}}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} & 0 & \pm\frac{im}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} \\ \pm\frac{im}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} & 0 & 1 \pm \frac{n\sin\omega^A_{\mathbf{k}}}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} & 0 \\ 0 & \pm\frac{im}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} & 0 & 1 \mp \frac{n\sin\omega^A_{\mathbf{k}}}{\sqrt{1-n^2\cos^2\omega^A_{\mathbf{k}}}} \end{pmatrix}. \tag{B15}$$

Finally, defining $U_{\mathbf{k}}$ such that $U_{\mathbf{k}}\tilde{A}_{\mathbf{k}}U_{\mathbf{k}}^\dagger = \mathrm{diag}(e^{-i\omega_{\mathbf{k}}^A}, e^{+i\omega_{\mathbf{k}}^A})$, one has

$$U_{\mathbf{k}}|\pm\rangle\langle\pm|U_{\mathbf{k}}^\dagger = \frac{1}{2}\left\{I \pm \frac{w(\mathbf{k})_r\sigma_x + w(\mathbf{k})_i\sigma_y + z(\mathbf{k})_i\sigma_z}{\sqrt{1-z(\mathbf{k})_r^2}}\right\}, \tag{B16}$$

where $x_{r,i}$ denote the real and imaginary part of x, respectively. Finally, we have

$$\Pi_{\mathbf{k}}^{\pm} = \frac{1}{2}\begin{pmatrix} 1 \mp \frac{nz(\mathbf{k})_i}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & \mp\frac{nw(\mathbf{k})^*}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & \pm\frac{im}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & 0 \\ \mp\frac{nw(\mathbf{k})}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & 1 \mp \frac{nz(\mathbf{k})_i}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & 0 & \pm\frac{im}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} \\ \pm\frac{im}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & 0 & 1 \pm \frac{nz(\mathbf{k})_i}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & \pm\frac{nw(\mathbf{k})^*}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} \\ 0 & \pm\frac{im}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & \pm\frac{nw(\mathbf{k})}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} & 1 \pm \frac{nz(\mathbf{k})_i}{\sqrt{1-n^2\cos^2\omega_{\mathbf{k}}^A}} \end{pmatrix}. \tag{B17}$$

Notice that the above expression is valid independently of the dimension and the particular solution of the unitarity equations.

APPENDIX C: DERIVATION OF THE WEYL AUTOMATON FOR $d = 1$ AND $d = 2$

In this Appendix we derive the unique solution to the unitarity equations (17) on $\mathbb{Z}^2$ and $\mathbb{Z}$.

It is easy to see that for $d = 2$ the only two Bravais lattices that are topologically inequivalent are the simple square and the hexagonal. We seek a QCA for minimal dimension $s = 2$. We remind the reader that Eqs. (A3) hold for any Bravais lattice in any space dimension, whence $A_{\mathbf{h}}$ and $A_{-\mathbf{h}}$ must have orthogonal supports and orthogonal ranges.

The unitarity conditions of Eq. (17) (omitting normalization) for both lattices read

$$A_{\mathbf{h}_i}^\dagger A_{-\mathbf{h}_i} = 0, \quad A_{\mathbf{h}_i}A_{-\mathbf{h}_i}^\dagger = 0,$$

$$A_{\mathbf{h}_i}^\dagger A_{\mathbf{h}_j} + A_{-\mathbf{h}_j}^\dagger A_{-\mathbf{h}_i} = 0, \tag{C1}$$

$$A_{\mathbf{h}_i}^\dagger A_{-\mathbf{h}_j} + A_{\mathbf{h}_j}^\dagger A_{-\mathbf{h}_i} = 0, \tag{C2}$$

$$A_{\mathbf{h}_i}A_{\mathbf{h}_j}^\dagger + A_{-\mathbf{h}_j}A_{-\mathbf{h}_i}^\dagger = 0, \tag{C3}$$

$$A_{\mathbf{h}_i}A_{-\mathbf{h}_j}^\dagger + A_{\mathbf{h}_j}A_{-\mathbf{h}_i}^\dagger = 0. \tag{C4}$$

Multiplying Eqs. (C3) and (C4) by $A_{\mathbf{h}_i}^\dagger$ on the left and by $A_{\mathbf{h}_j}$ on the right and exploiting Eq. (C2), we obtain

$$[|A_{\mathbf{h}_i}|^2, |A_{\pm\mathbf{h}_j}|^2] = 0 \quad \forall\, i,j. \tag{C5}$$

By condition Eq. (C1) we see that $\alpha_+ = \alpha_- =: \alpha$. We can then label the vertices in such a way that the identities

$$A_{\mathbf{h}_i} = \alpha V_i M, \quad A_{-\mathbf{h}_i} = \alpha V_i (I - M) \tag{C6}$$

hold, where $M = |\eta_{+,i}\rangle\langle\eta_{+,i}|$. Notice, however, that the relabeling may not correspond to a unitary conjugation, so we have to check *a posteriori* that the relabeled automaton is equivalent to the original one. Indeed, as we will see, the relabeled automaton is related to the original one by transposition.

Now the conditions Eq. (C1) are equivalent to

$$MV_i^\dagger V_j M + (I-M)V_j^\dagger V_i (I-M) = 0, \tag{C7}$$

namely,

$$MV_i^\dagger V_j M = (I-M)V_j^\dagger V_i (I-M) = 0. \tag{C8}$$

Defining $\sigma_z := M - (I - M)$, we then have

$$V_i^\dagger V_j = \nu_{ij}\mathbf{n}_{ij}\cdot\boldsymbol{\sigma}, \tag{C9}$$

with $\mathbf{n}_{ij}$ lying on the plane xy. Similarly, the conditions in Eq. (C2) read

$$MV_i^\dagger V_j (I-M) + MV_j^\dagger V_i (I-M) = 0, \tag{C10}$$

namely, $\nu_{ij} = -\nu_{ij}^* = \pm i$.

1. Hexagonal lattice

It is easy to show that the hexagonal lattice is incompatible with unitarity. In fact, since

$$V_1^\dagger V_3 = V_1^\dagger V_2 V_2^\dagger V_3, \tag{C11}$$

we have

$$\mathbf{n}_{12}\cdot\mathbf{n}_{23} = 0, \quad \mathbf{n}_{13} = -i\mathbf{n}_{12}\times\mathbf{n}_{23}, \tag{C12}$$

which is impossible to satisfy with all $\mathbf{n}_{ij}$'s lying on the xy plane. Therefore, there exists no QCA for the $s = 2$ on a hexagonal lattice.

2. Square lattice

On the other hand, for the square lattice we have

$$V_1^\dagger V_2 = i\mathbf{n}\cdot\boldsymbol{\sigma}, \tag{C13}$$

and then

$$\tilde{A}_{\mathbf{k}} = A_{\mathbf{h}_1}e^{ik_1} + A_{-\mathbf{h}_1}e^{-ik_1} + A_{\mathbf{h}_2}e^{ik_2} + A_{-\mathbf{h}_2}e^{-ik_2}, \tag{C14}$$

which is equal to

$$\tilde{A}_{\mathbf{k}} = \alpha V_1\{Me^{ik_1} + (I-M)e^{-ik_1} + i\mathbf{n}\cdot\boldsymbol{\sigma}[Me^{ik_2} + (I-M)e^{-ik_2}]\}, \tag{C15}$$

namely,

$$\tilde{A}_{\mathbf{k}} = \alpha V_1\begin{pmatrix} e^{ik_1} & -\nu^* e^{-ik_2} \\ \nu e^{ik_2} & e^{-ik_1}\end{pmatrix}, \tag{C16}$$

where $|\nu|^2 = 1$. Now, if we impose the condition Eq. (19) we simply have

$$V_1^\dagger = \alpha \begin{pmatrix} 1 & -\nu^* \\ \nu & 1 \end{pmatrix}, \tag{C17}$$

which implies $\alpha = 1/\sqrt{2}$ and

$$\tilde{A}_{\mathbf{k}} = \frac{1}{2}\begin{pmatrix} e^{ik_1} + e^{ik_2} & \nu^*(e^{-ik_1} - e^{-ik_2}) \\ -\nu(e^{ik_1} - e^{ik_2}) & e^{-ik_1} + e^{-ik_2} \end{pmatrix}. \tag{C18}$$

Notice also that the automaton in Eq. (C18) for a given $\nu = r + ij$ can be obtained from the automaton with $\nu = -i$ just by a fixed rotation around σ_z, and then we now refer to the choice $\omega = -i$. We can express such automaton as

$$\begin{aligned}\tilde{A}_{\mathbf{k}} = \tfrac{1}{2}\{&(c_1 + c_2)I - i[(c_1 - c_2)\sigma_x \\ &+ (s_1 - s_2)\sigma_y - (s_1 + s_2)\sigma_z]\},\end{aligned} \tag{C19}$$

where $c_i = \cos k_i$ and $s_i = \sin k_i$. However, in order to obtain in the relativistic limit the canonical form of the Weyl equation, we change the representation so that

$$\begin{aligned}\tilde{A}_{\mathbf{k}} = \tfrac{1}{2}\{&(c_1 + c_2)I - i[(s_1 + s_2)\sigma_x \\ &+ (s_1 - s_2)\sigma_y + (c_1 - c_2)\sigma_z]\},\end{aligned} \tag{C20}$$

corresponding to the unitary mapping $(\sigma_x,\sigma_y,\sigma_z) \mapsto (\sigma_z,\sigma_y, -\sigma_x)$. In this representation, the solution corresponds to the expression for the automaton

$$\begin{aligned}\tilde{A}_{\mathbf{k}} &= \frac{1}{4}\begin{pmatrix} z(\mathbf{k}) & iw(\mathbf{k})^* \\ iw(\mathbf{k}) & z(\mathbf{k})^* \end{pmatrix}, \\ z(\mathbf{k}) &:= \zeta^*(e^{ik_1} + e^{-ik_1}) + \zeta(e^{ik_2} + e^{-ik_2}), \\ w(\mathbf{k}) &:= \zeta(e^{ik_1} - e^{-ik_1}) + \zeta^*(e^{ik_2} - e^{-ik_2}), \\ \zeta &:= \frac{1+i}{4},\end{aligned} \tag{C21}$$

which can be written as

$$\tilde{A}_{\mathbf{k}}^{\pm} = I d_{\mathbf{k}} - i\boldsymbol{\sigma}\cdot\mathbf{a}_{\mathbf{k}}, \tag{C22}$$

where

$$\begin{aligned}(a_{\mathbf{k}})_x &:= s_x c_y, \quad (a_{\mathbf{k}})_y := c_x s_y, \\ (a_{\mathbf{k}})_z &:= s_x s_y, \quad d_{\mathbf{k}} := c_x c_y,\end{aligned} \tag{C23}$$

where we introduced the representation

$$k_x := \frac{k_1 + k_2}{\sqrt{2}}, \quad k_y := \frac{k_1 - k_2}{\sqrt{2}}. \tag{C24}$$

The symbols c_i and s_i denote $\cos\frac{k_i}{\sqrt{2}}$ and $\sin\frac{k_i}{\sqrt{2}}$, respectively. The dispersion relation is

$$\omega_{\mathbf{k}}^A = \arccos(c_x c_y). \tag{C25}$$

Notice, however, that the form (C20) is manifestly covariant for the cyclic transitive group $L = \{e,a\}$ generated by the transformation a that exchanges $\mathbf{h}_1$ and $\mathbf{h}_2$, with representation given by the rotation by π around the x axis.

If we now consider the possible relabeling $\mathbf{h}_2 \mapsto -\mathbf{h}_2$, using Eq. (C20) we can easily verify that it corresponds to the transformation $(\sigma_x,\sigma_y,\sigma_z) \mapsto (\sigma_y,\sigma_x,\sigma_z)$, which modulo unitary conjugation amounts to transposition.

The only possible local coupling of two Weyl automata is obtained, as for the 3D case, as

$$\tilde{E}_{\mathbf{k}} = \begin{pmatrix} n\tilde{A}_{\mathbf{k}} & imI \\ imI & n\tilde{A}_{\mathbf{k}}^\dagger \end{pmatrix}, \tag{C26}$$

with $n^2 + m^2 = 1$.

As in the 3D case, we can write the automaton $\tilde{E}_{\mathbf{k}}$ in terms of the γ matrices as

$$\tilde{E}_{\mathbf{k}} = I d_{\mathbf{k}} - i\gamma^0\boldsymbol{\gamma}\cdot\mathbf{a}_{\mathbf{k}} + im\gamma^0, \tag{C27}$$

where $d_{\mathbf{k}}^E = n d_{\mathbf{k}}^A$ and $\mathbf{a}_{\mathbf{k}}^E = n\mathbf{a}_{\mathbf{k}}^A$.

We also define the Cartesian components of $\mathbf{k}$ as follows:

$$k_x := \frac{1}{\sqrt{2}}(k_1 + k_2), \quad k_y := \frac{1}{\sqrt{2}}(k_1 - k_2). \tag{C28}$$

[1] R. P. Feynman, A. R. Hibbs, and D. F. Styer, *Quantum Mechanics and Path Integrals*, Dover Books on Physics Series (Dover, New York, 2005).
[2] T. Nakamura, J. Math. Phys. **32**, 457 (1991).
[3] I. Bialynicki-Birula, Phys. Rev. D **49**, 6920 (1994).
[4] D. A. Meyer, J. Stat. Phys. **85**, 551 (1996).
[5] J. Yepez, Quantum Inf. Process. **4**, 471 (2006).
[6] J. von Neumann, *Theory of Self-reproducing Automata* (University of Illinois Press, Urbana and London, 1966).
[7] T. Toffoli and N. Margolus, *Cellular Automata Machines* (MIT Press, Cambridge, MA, 1987).
[8] R. P. Feynman, Int. J. Theor. Phys. **21**, 467 (1982).
[9] J. A. Wheeler, Int. J. Theor. Phys. **21**, 557 (1982).
[10] Edited by A. J. G. Hey, *Feynman and Computation: Exploring the Limits of Computers* (Perseus Books, Reading, MA, 1999).
[11] G. 't Hooft, Nucl. Phys. B **342**, 471 (1990).
[12] Stephen Wolfram, *A New Kind of Science* (Wolfram Media, Champaign, IL, 2002), Vol. 5.
[13] G. M. D'Ariano, AIP Conf. Proc. **1232**, 3 (2010).
[14] G. M. D'Ariano, Phys. Lett. A **376**, 697 (2012).
[15] G. M. D'Ariano, Il Nuovo Saggiatore **28**, 13 (2012).
[16] M. Kuhlmann, in *The Stanford Encyclopedia of Philosophy*, edited by E. N. Zalta (Stanford University, Stanford, CA, 2012).
[17] D. B. Malament, in *Perspectives on Quantum Reality*, edited by Rob Clifton, The University of Western Ontario Series in Philosophy of Science Vol. 57 (Springer, Netherlands, 1996), pp. 1–10.
[18] R. Clifton and H. Halvorson, in *Quantum Entanglement: Selected Papers*, edited by Rob Clifton, J. Butterfield, and H. Halvorson (Oxford University Press, Oxford, UK, 2004), p. 225.
[19] B. Zwiebach, *A First Course in String Theory* (Cambridge University Press, Cambridge, UK, 2004).
[20] K. Becker, M. Becker, and J. H. Schwarz, *String Theory and M-Theory: A Modern Introduction* (Cambridge University Press, Cambridge, 2006).
[21] T. Jacobson, Phys. Rev. Lett. **75**, 1260 (1995).

[22] E. Verlinde, J. High Energy Phys. 04 (2011) 029.
[23] G. Amelino-Camelia, Int. J. Mod. Phys. D **11**, 1643 (2002).
[24] G. Amelino-Camelia and T. Piran, Phys. Rev. D **64**, 036005 (2001).
[25] J. Magueijo and L. Smolin, Phys. Rev. Lett. **88**, 190403 (2002).
[26] J. Magueijo and L. Smolin, Phys. Rev. D **67**, 044017 (2003).
[27] M. Moyer, Sci. Am. **306**, 30 (2012).
[28] Craig J. Hogan, Phys. Rev. D **85**, 064007 (2012).
[29] I. Pikovski, M. R. Vanner, M. Aspelmeyer, M. Kim, and C. Brukner, Nat. Phys. **8**, 393 (2012).
[30] G. Amelino-Camelia, C. Lämmerzahl, F. Mercati, and G. M. Tino, Phys. Rev. Lett. **103**, 171302 (2009).
[31] A. Bibeau-Delisle, A. Bisio, G. M. D'Ariano, P. Perinotti, and A. Tosini, arXiv:1310.6760.
[32] G. Grössing and A. Zeilinger, Complex Syst. **2**, 197 (1988).
[33] A. Ambainis, E. Bach, A. Nayak, A. Vishwanath, and J. Watrous, in *Proceedings of the Thirty-third Annual ACM Symposium on Theory of Computing* (ACM, New York, 2001), pp. 37–49.
[34] B. Schumacher and R. F. Werner, arXiv:quant-ph/0405174.
[35] P. L. Knight, E. Roldán, and J. E. Sipe, J. Mod. Opt. **51**, 1761 (2004).
[36] P. Arrighi, V. Nesme, and R. Werner, J. Comput. Syst. Sci. **77**, 372 (2011).
[37] D. Gross, V. Nesme, H. Vogts, and R. F. Werner, Comm. Math. Phys. **310**, 419 (2012).
[38] S. B. Bravyi and A. Y. Kitaev, Ann. Phys. **298**, 210 (2002).
[39] G. M. D'Ariano, F. Manessi, P. Perinotti, and A. Tosini, Int. J. Mod. Phys. A **29**, 1430025 (2014).
[40] G. M. D'Ariano, F. Manessi, P. Perinotti, and A. Tosini, EPL **107**, 20009 (2014).
[41] Mikhael Gromov, in *Proceedings of the International Congress of Mathematicians, Aug. 16–24 1983, Warszawa* (PWN-Polish Scientific Publishers, Warszawa, 1984), p. 385.
[42] M. R. Bridson, in *The Princeton Companion to Mathematics*, edited by T. Gowers, J. Barrow-Green, and I. Leader (De Gruyter, Berlin, 1949), p. 431.
[43] Y. de Cornulier, R. Tessera, and A. Valette, Geom. Funct. Anal. **17**, 770 (2007).
[44] A. Bisio, G. M. D'Ariano, and A. Tosini, arXiv:1212.2839.
[45] H. B. Nielsen and M. Ninomiya, Phys. Lett. B **105**, 219 (1981).
[46] A. Pelissetto, Ann. Phys. **182**, 177 (1988).