Isotropic quantum walks on lattices and the Weyl equation

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We present a thorough classification of the isotropic quantum walks on lattices of dimension $d = 1,2,3$ with a coin system of dimension $s = 2$. For $d = 3$ there exist two isotropic walks, namely, the Weyl quantum walks presented in the work of D'Ariano and Perinotti [G. M. D'Ariano and P. Perinotti, Phys. Rev. A **90**, 062106 (2014)], resulting in the derivation of the Weyl equation from informational principles. The present analysis, via a crucial use of isotropy, is significantly shorter and avoids a superfluous technical assumption, making the result completely general.

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I. INTRODUCTION

Recently the possibility of implementing actual quantum simulations of quantum fields [1–4] has been accompanied by novel approaches to foundations of the theory [5–8], including its derivation from informational principles [9,10] and the recovery of its Lorentz covariance [11]. This has provided progress in the research based on the idea originally proposed by Feynman [12] of recovering physics as pure quantum information processing. Deriving quantum field theory from just denumerable quantum systems provides an emergent notion of space-time, with no prior background. This suggests that the approach may be promising for future development of quantum theories of gravity.

The mathematical formalization of the discrete quantum algorithm running a quantum field dynamics is provided by the notion of a quantum cellular automaton [13–15]. A quantum cellular automaton is a unitary homogeneous evolution of the algebra of local observables that preserves locality. When the automaton is linear in the local algebra generators, the cellular automaton is usually referred to as a quantum walk (QW) [16–18] and is suited for the description of the free field theory for a fixed number of particles.

A quantum walk on a graph represents a coherent counterpart of a classical random walk on the same graph. In the derivation of Ref. [9] it was proved that, if one assumes homogeneity of the evolution, the graph must be the Cayley graph of a group G. When the graph corresponds to a free Abelian group $G \cong \mathbb{Z}^d$, one finds the two Weyl QWs (one for the left- and one for the right-handed mode), recovering the Weyl equation in $d + 1$ dimensions for $d = 1,2,3$. An alternative derivation of the Weyl QWs for $d = 3$ on the bcc lattice was recently presented in Ref. [19]. In Ref. [9] the derivation of the Weyl QWs exploited the technical assumption that there is a quasi-isometry [20] of the Cayley graph in a Euclidean manifold such that no vertex can lie within the sphere of nearest neighbors. On the other hand, most of the derivation did not use the isotropy principle. In the present paper, on the contrary, we exploit the isotropy principle from the very beginning of the derivation, thus avoiding the above assumption and making the classification of the isotropic QWs on $\mathbb{Z}^d$ completely general. In the present paper the derivation of the Weyl QWs is included in a complete classification of isotropic QWs on lattices of dimension $d = 1,2,3$ with a coin system of dimension $s = 2$. The result exploits the isotropy notion of Ref. [9], which is extended in this paper in order to account for groups with generators of different orders. We will introduce a technique to construct the Cayley graphs of a given group G supporting an isotropic QW. Remarkably, the Cayley graph is unique for each dimension $d = 1,2,3$.

The paper is organized as follows. In Sec. II we review the notion of Cayley graph of a group G and define QWs on Cayley graphs, introducing the definition of isotropy and its main properties. In Sec. III we review the theory of QWs on free Abelian groups. In Sec. IV we select the possible Cayley graphs according to a necessary condition for a QW to be isotropic. In Sec. V we prove a second necessary condition for isotropy that is used in the Appendix to refine the selection of Cayley graphs and we solve the unitarity condition on the selected Cayley graphs for $d = 1,2,3$, finding the two Weyl QWs. Section VI summarizes the paper. In the Appendix we report technical proofs and details.

II. ISOTROPIC QWS ON CAYLEY GRAPHS

We now define the QW on a Cayley graph $\Gamma(G,S_+)$ of a group G, with generating set S_+. A generating set $S_+ \subseteq G$ is a set of elements of G such that all the elements of the group can be expressed as words of elements of S_+ along with their inverses. The Cayley graph is a colored directed graph with the elements of G as vertices and the elements of S_+ as edges: A color is associated with each generator $h \in S_+$ and two vertices $g,g' \in G$ are connected by the colored edge $h \in S_+$ if $g' = gh$, with the arrow directed from g to g'. In the following we will take $|S_+| < \infty$, namely, the group G is finitely generated. The Cayley graph of a group can be defined by giving a presentation, namely, choosing a set of generators (an alphabet) and a set of relators, i.e., a set of words which are equal to the identity of G. This completely specifies a unique group G. The cardinality of the group G can be finite or infinite, depending on its relators; however, the most interesting case in the present context is that of a finitely presented infinite group.

Let $\{|g\rangle\}_{g\in G}$ be an orthonormal basis for $\ell^2(G)$. The right-regular representation T of G is defined as

$$T_g|g'\rangle := |g'g^{-1}\rangle. \tag{1}$$

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A QW on the Cayley graph $\Gamma(G,S_+)$ of the group G is a unitary operator A on $\ell^2(G)\otimes\mathbb{C}^s$, with $1\leqslant s<\infty$, that can be written as

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

where $S=S_+\cup S_-$, $S_-=S_+^{-1}$ is the set of inverses of S_+, and $\{A_h\}_{h\in S}\subseteq\mathbb{M}_s(\mathbb{C})$ are the so-called transition matrices of the QW. It is worth mentioning that also other constructions of QWs have been given in the literature, for example, QWs such that the coin system is generated by the set of edges of the underlying graph (see, e.g., Ref. [21], and Ref. [22] for an overview).

Generally, we will consider also self-transitions, corresponding to the inclusion of the identity $e\in G$ in the generating set, which is then given by $S\equiv S_+\cup S_-\cup\{e\}$. In the following, for each group G considered, we will assume $A_h\neq 0$ for all $h\in S_+\cup S_-$, whereas in general we allow for the case $A_e=0$. We also denote by $S_+^n\subseteq S_+$ the set of generators of order $n\geqslant 2$, i.e., n is the smallest integer such that $h^n=e$. Notice that the most common case is that of $n=+\infty$.

For the purpose of introducing the concept of isotropic QWs, we recall that a graph automorphism is defined as a bijective map of the vertices that preserves the set of edges. For a Cayley graph this means that the automorphism l is such that if $g'=gh$, then $l(g')=l(g)h'$, with $g,g'\in G$ and $h,h'\in S_+$. Then an automorphism of the Cayley graph can be expressed as a permutation λ of the set of colors S_+, where for every $g\in G$ and $h\in S_+$ one has $l(gh)=l(g)\lambda(h)$ for some permutation λ of S_+. Let us denote by Λ a group of permutations of the elements of S_+.

Definition 1. A QW on $\Gamma(G,S_+)$ is called isotropic with respect to S_+ if there exists a group L of automorphisms of $\Gamma(G,S_+)$ that can be expressed as a permutation of the colors S_+ such that the evolution operator of the QW is L covariant, i.e., there exists a projective unitary representation U over $\mathbb{C}^s$ of L such that

$$A_{\lambda(h)}=U_lA_hU_l^\dagger\quad\forall l\in L,\forall h\in S_+,$$

where $\lambda\in\Lambda$, and such that the action of Λ is transitive on each subset S_+^n.

The previous definition guarantees that the group of local changes of basis representing the isotropy group L, which is a group of automorphisms of the graph, acts just as a permutation of the transition matrices, implying that all the directions are dynamically equivalent. To satisfy homogeneity, one has to demand also the following condition:[1]

$$[U_l,A_h]\neq 0\quad\forall h\in S_+,\forall l\in L:l(h)\neq h.\qquad(2)$$

Indeed, two transition matrices associated with different generators must be distinct. In particular, this implies that if L does not contain nontrivial elements stabilizing all the $h\in S$, then the representation U must be faithful (otherwise it would contain at least one nontrivial element represented as I_s).

Propostion 1. The automorphisms of the Cayley graph $\Gamma(G,S_+)$ are also automorphisms of G.

Proof. Consider the action of arbitrary elements $l\in L$ on the graph vertices. We have

$$\lambda(h)=l(h)=l(eh)=e\lambda(h)\quad\forall h\in S_+,$$

and since $l(gh)=l(g)\lambda(h)\ \forall g\in G$, then $l(e)=e$. The same holds $\forall h\in S_-$. Moreover,

$$l(hh')=l(h)\lambda(h')\equiv l(h)l(h')\quad\forall h,h'\in S.$$

Iterating, in general we obtain

$$l(h_1\cdots h_p)=l(h_1)\cdots l(h_p)\quad\forall h_1,\ldots,h_p\in S,\qquad(3)$$

and since S is a set of generators for G, this amounts to

$$l(gg')=l(g)l(g')\quad\forall g,g'\in G.$$

Accordingly, L is a group automorphism of G. ■

The isotropy conditions corresponds to the covariance

$$A=\sum_{h\in S}T_h\otimes A_h=\sum_{h\in S}T_{l(h)}\otimes U_lA_hU_l^\dagger\quad\forall l\in L.\qquad(4)$$

The covariance condition (4) and the transitivity of Λ on each S_+^n imply, by linear independence of the T_h, that every S_+^n is invariant under some subgroup $L^n\leqslant L$. In fact, any S_+^n is the orbit of an arbitrary generator $h_1^{(n)}\in S_+^n$ under L^n, denoted by $\mathcal{O}_{L^n}(h_1^{(n)})$.

Proposition 2. The isotropy group L is a finite subgroup of $\mathrm{Aut}(G)$.

Proof. By Proposition 1 the isotropy group L is a group of automorphisms of G. By Eq. (3), $L\cong\Lambda$, hence L is finite. ■

Corollary 1. Each subgroup $L^n\leqslant L$ is isomorphic to a finite permutation group acting transitively on S_+^n.

Corollary 2. If all generators have the same order, L is isomorphic to a finite permutation group acting transitively on S_+.

By Eq. (4) one can always choose the projective unitary representation U with unit determinant, namely, $U_l\in SU(s)$ $\forall l\in L$. Notice that, by definition of isotropy, either S_+^n does not contain the inverse of any of its elements or it coincides with the whole set $S^n:=S_+^n\cup S_-^n$.

In the following we will consider the isotropic QWs on $\Gamma(G,S_+)$ with $s=2$ and $G\cong\mathbb{Z}^d$ with $d=1,2,3$. For $d=3$ we discover that there are two QWs (modulo discrete symmetries) that for large-scales give the two Weyl equations, one for the left- and one for the right-handed mode. In Ref. [9] it is shown that, coupling two Weyl QWs in the only possible way consistent with the above requirements (specifically locality), the resulting QW is unique (modulo discrete symmetries) and describes exactly the Dirac equation for large scales.

III. QUANTUM WALKS ON CAYLEY GRAPHS OF $\mathbb{Z}^d$

Since we are considering Abelian groups, we will denote the group elements as usual with the boldface vector notation as $\mathbf{n}\in G$ and the generators as $\mathbf{h}\in S$. Moreover, we will use the additive notation for the group composition and 0 for the identity element. The space $\ell^2(G)$ will be the span of $\{|\mathbf{n}\rangle\}_{\mathbf{n}\in G}$

[1]The homogeneity requirement defined in Ref. [9] should be completed upon requiring that any two nodes remain distinguishable from the point of view of a third node. For details we will refer to Ref. [23]. Equation (2) follows from this definition.

and the generators $\mathbf{h}$ are represented by the operators

$$T_{\mathbf{h}} := \sum_{\mathbf{n}\in G} |\mathbf{n}+\mathbf{h}\rangle\langle\mathbf{n}|.$$

We now treat the elements of G as vectors in $\mathbb{R}^d$. Generally, the elements of S are linearly dependent. We introduce all the sets $D_n \subseteq S_+$ of linearly independent elements

$$D_n := \{\mathbf{h}_{i_1},\ldots,\mathbf{h}_{i_d}\},$$

where n labels the specific subset. For every D_n we construct the dual set $\tilde{D}_n$ defined by

$$\tilde{D}_n := \{\tilde{\mathbf{h}}_1^{(n)},\ldots,\tilde{\mathbf{h}}_d^{(n)}\},$$

where

$$\tilde{\mathbf{h}}_l^{(n)} \cdot \mathbf{h}_{i_m} = \delta_{lm}.$$

Now we define the set

$$\tilde{D} := \bigcup_n \tilde{D}_n.$$

The Brillouin zone $B \subseteq \mathbb{R}^d$ is defined as the polytope

$$B = \bigcap_{\tilde{\mathbf{h}}\in\tilde{D}} \{\mathbf{k}\in\mathbb{R}^d \mid -\pi|\tilde{\mathbf{h}}|^2 \leqslant \mathbf{k}\cdot\tilde{\mathbf{h}} \leqslant \pi|\tilde{\mathbf{h}}|^2\}.$$

The unitary operator of the QW is given by

$$A = \sum_{\mathbf{n}\in G}\sum_{\mathbf{h}\in S} |\mathbf{n}+\mathbf{h}\rangle\langle\mathbf{n}| \otimes A_{\mathbf{h}}. \tag{5}$$

One has $[A, T_{\mathbf{h}}\otimes I_s] = 0$. The unitary irreducible representations are one dimensional and are classified by the joint eigenvectors of $T_{\mathbf{h}}$,

$$T_{\mathbf{h}_i}|\mathbf{k}\rangle =: e^{-i\mathbf{k}\cdot\mathbf{h}_i}|\mathbf{k}\rangle,$$

where

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

Notice that

$$\langle\mathbf{k}|\mathbf{k}'\rangle = \frac{1}{|B|}\sum_{\mathbf{n}\in G} e^{i(\mathbf{k}-\mathbf{k}')\cdot\mathbf{n}} = \delta_{2\pi}(\mathbf{k}-\mathbf{k}').$$

Translation invariance of the QW in Eq. (5) then implies the following form for the unitary evolution operator:

$$A = \int_B d\mathbf{k} |\mathbf{k}\rangle\langle\mathbf{k}| \otimes A_{\mathbf{k}},$$

where the the matrix

$$A_{\mathbf{k}} = \sum_{\mathbf{h}\in S} e^{i\mathbf{h}\cdot\mathbf{k}} A_{\mathbf{h}} \tag{6}$$

is unitary for every $\mathbf{k}$. Notice that $A_{\mathbf{k}}$ is a matrix polynomial in $e^{i\mathbf{h}\cdot\mathbf{k}}$. The unitarity conditions on $A_{\mathbf{k}}$ for all $\mathbf{k}\in B$ then read

$$\sum_{\mathbf{h}\in S} A_{\mathbf{h}}A_{\mathbf{h}}^\dagger = \sum_{\mathbf{h}\in S} A_{\mathbf{h}}^\dagger A_{\mathbf{h}} = I_s, \tag{7}$$

$$\sum_{\mathbf{h}-\mathbf{h}'=\mathbf{h}''} A_{\mathbf{h}}A_{\mathbf{h}'}^\dagger = \sum_{\mathbf{h}-\mathbf{h}'=\mathbf{h}''} A_{\mathbf{h}'}^\dagger A_{\mathbf{h}} = 0. \tag{8}$$

Equations (7) and (8) are a set of necessary and sufficient conditions for the unitarity of the time evolution, since they can be derived just imposing that the matrix $A_{\mathbf{k}}$ is unitary. As explained in Sec. II, the requirement of isotropy for the QW needs the existence of a group that acts transitively over the generator set S_+ with a faithful projective unitary representation that satisfies Eq. (4). Notice that one has the identity

$$(I\otimes A_{\mathbf{k}=0}^\dagger)A = \sum_{\mathbf{h}\in S} T_{\mathbf{h}}\otimes A'_{\mathbf{h}},$$

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

$$\sum_{\mathbf{h}\in S} A_{\mathbf{h}} = I_s, \tag{9}$$

as explained in the following. Indeed, the isotropy requirement implies that $A_{\mathbf{k}=0}$ commutes with the representation of the isotropy group L, whence we can classify the QW by requiring the identity (9) and then multiplying the QW operator A on the left by $(I\otimes V)$, with V unitarily commuting with the representation of L. In the case that the representation is irreducible, then by the Schur lemma we have only $V = I_s$.

From now on we will restrict our study to $s = 2$, which corresponds to the simplest nontrivial QW in the case of G Abelian. Indeed, in Ref. [24] it was proved that if G is an arbitrary Abelian group and $s = 1$ (scalar QW case), then the evolution is trivial.

IV. IMPOSING ISOTROPY: ADMISSIBLE CAYLEY GRAPHS OF $\mathbb{Z}^d$

In this section we investigate how the isotropy assumption restricts the possible presentations of $G \cong \mathbb{Z}^d$. By Proposition 2, the isotropy groups are finite subgroups $L < \mathrm{Aut}(\mathbb{Z}^d) \cong \mathrm{GL}(d,\mathbb{Z})$: Their action, by Corollary 2, is defined to be transitive on the generating set S_+ and then is extended on all $\mathbb{Z}^d$ by linearity. Indeed, the generating set S_+ is the orbit of an arbitrary vector $\mathbf{v}\in\mathbb{R}^d$ under the action of a finite subgroup $L < \mathrm{GL}(d,\mathbb{Z})$.

Let M be a representation on integers of L (so that $M_l M_f = M_{lf}$ for $l,f\in L$) and let us define the matrix $P := \sum_{l\in L} M_l^T M_l$. For every $f\in L$ we have

$$\begin{aligned} PM_f &= \sum_{l\in L} M_l^T M_{lf} = \sum_{l'\in L} M_{l'f^{-1}}^T M_{l'} \\ &= \sum_{l'\in L} (M_{l'}M_{f^{-1}})^T M_{l'} = M_{f^{-1}}^T P. \end{aligned} \tag{10}$$

Moreover, being a sum of positive operators, P is also positive. Then, for $|\eta\rangle\in\ker P$, $\langle\eta|P|\eta\rangle = \sum_{l\in L}\langle\eta|M_l^T M_l|\eta\rangle = 0$ implies that $M_l|\eta\rangle = 0\ \forall l\in L$, namely, $|\eta\rangle = 0$ since all M_l are invertible. Thus P has a trivial kernel and we can define the invertible change of representation

$$\tilde{M}_l := P^{1/2}M_l P^{-1/2}. \tag{11}$$

Using the definition of P and property (10), we obtain

$$\begin{aligned} \tilde{M}_l{}^T\tilde{M}_l &= P^{-1/2}M_l^T P M_l P^{-1/2} \\ &= P^{-1/2}M_l^T M_{l^{-1}}^T P P^{-1/2} = I. \end{aligned}$$

This means that, as long as one embeds the Cayley graphs in $\mathbb{R}^d$, L can always be represented orthogonally. Notice that the representation $\tilde{M}$ is in general on real numbers, namely, $\{\tilde{M}_l\}_{l\in L} \subset \mathbb{O}(d,\mathbb{R})$ [from now on we denote it just by O(d)].

As one can find in Refs. [25,26], the finite subgroups of GL($d,\mathbb{Z}$) which are also subgroups of O(d) are isomorphic to (i) $d = 3$ for $\mathbb{Z}_n$ and D_n with $n \in \{1,2,3,4,6\}$, A_4 and S_4, and the direct products of all the previous groups with $\mathbb{Z}_2$; (ii) $d = 2$ for $\mathbb{Z}_n$ and D_n with $n \in \{1,2,3,4,6\}$; and (iii) $d = 1$ for $\{e\}$ and $\mathbb{Z}_2$. Accordingly, our cases of interest $d = 1,2,3$ can be treated together, considering just $d = 3$. We notice that for $d = 1,2$ the finite subgroups of GL($d,\mathbb{Z}$) coincide with those of O(d), while for $d = 3$ we are restricted to those finite subgroups of GL($3,\mathbb{Z}$) that are also subgroups of O(3).

A given generating set for $\mathbb{Z}^d$ satisfying the definition of isotropy can be constructed orbiting a vector in $\mathbb{R}^d$ under the aforementioned finite subgroups in O(d). Accordingly, given a presentation for $\mathbb{Z}^d$, if the associated Cayley graph satisfies isotropy then one can represent the generators having all the same Euclidean norm, namely, they lie on a sphere centered at the origin: They form the orbit, which we will denote by $\mathcal{O}_L(\mathbf{v})$, of an arbitrary d-dimensional real vector $\mathbf{v}$ under the action of a finite subgroup $L < \mathrm{GL}(d,\mathbb{Z})$ represented in O(d).

In the Appendix we will consider the orbit of a vector $\mathbf{v} \in \mathbb{R}^3$ under the real, orthogonal, and three-dimensional faithful representations of L. Indeed, if we took into account also unfaithful representations, these would have a nontrivial kernel, which is a normal subgroup, and the effective action on $\mathbf{v}$ would be given by a faithful representation of the quotient group. Inspecting the subgroup structure of the finite subgroups of GL($3,\mathbb{Z}$), one can check that all the possible quotients are themselves finite subgroups of GL($3,\mathbb{Z}$).[2] Thus, the case of unfaithful representations is already considered as long as we take into account the faithful ones.

V. THE QWS WITH MINIMAL COMPLEXITY: THE WEYL QUANTUM WALKS

In the following $X = V|X|$ will define the polar decomposition of the operator X, with $|X| := \sqrt{X^\dagger X}$ the modulus of X and V unitary. Thus we will write the transition matrix as

$$A_{\mathbf{h}} = V_{\mathbf{h}}|A_{\mathbf{h}}|. \tag{12}$$

From Eq. (8) with $\mathbf{h}'' = 2\mathbf{h}$ it follows that $A_{\mathbf{h}}A^\dagger_{-\mathbf{h}} = 0$, namely, $|A_{\mathbf{h}}\|A^\dagger_{-\mathbf{h}}| = 0$. By definition the transition matrices are nonnull, hence $|A_{\mathbf{h}}|$ and $|A_{-\mathbf{h}}|$ must have orthogonal supports, and for $s = 2$ they must then be rank-1. Thus they can be written as

$$A_{\mathbf{h}} =: \alpha_{\mathbf{h}} V_{\mathbf{h}}|\eta_{\mathbf{h}}\rangle\langle\eta_{\mathbf{h}}|, \quad A_{-\mathbf{h}} =: \alpha_{-\mathbf{h}} V_{-\mathbf{h}}|\eta_{-\mathbf{h}}\rangle\langle\eta_{-\mathbf{h}}|, \tag{13}$$

where $\{|\eta_{+\mathbf{h}}\rangle,|\eta_{-\mathbf{h}}\rangle\}$ is an orthonormal basis and $\alpha_{\mathbf{h}} > 0$. By the isotropy requirement we have that for all $\mathbf{h},\mathbf{h}'$, $\alpha_{\pm\mathbf{h}} = \alpha_{\pm\mathbf{h}'} =: \alpha_\pm$. Furthermore, it is easy to see that we can choose $V_{\mathbf{h}} = V_{-\mathbf{h}}$ for every $\mathbf{h}$.[3]

Denoting the elements of $S_\pm$ by $\pm\mathbf{h}_i$, suppose that there exists a subgroup $K \leqslant L$ such that, for some $\mathbf{h}_1 \in S_+$, $\forall \mathbf{h}_i,\mathbf{h}_j \in \mathcal{O}_K(\mathbf{h}_1)$ with $\mathbf{h}_i \neq \mathbf{h}_j$, and for $\mathbf{h}_l,\mathbf{h}_m \in \{\mathbf{0},\mathcal{O}_L(\mathbf{h}_1)\}$, one has

$$\mathbf{h}_i - \mathbf{h}_j = \mathbf{h}_l - \mathbf{h}_m \iff (\mathbf{h}_i = \mathbf{h}_l) \vee (\mathbf{h}_i = -\mathbf{h}_m). \tag{14}$$

Then a second set of equations from conditions (8) is

$$A_{\mathbf{h}_1}A^\dagger_{\mathbf{h}_j} + A_{-\mathbf{h}_j}A^\dagger_{-\mathbf{h}_1} = 0, \tag{15}$$

$$A^\dagger_{\mathbf{h}_1}A_{\mathbf{h}_j} + A^\dagger_{-\mathbf{h}_j}A_{-\mathbf{h}_1} = 0. \tag{16}$$

Multiplying Eq. (15) by $A^\dagger_{\mathbf{h}_j}$ on the left or by $A_{\mathbf{h}_1}$ on the right, we obtain

$$A^\dagger_{\mathbf{h}_j}A_{\mathbf{h}_1}A^\dagger_{\mathbf{h}_j} = A_{\mathbf{h}_1}A^\dagger_{\mathbf{h}_j}A_{\mathbf{h}_1} = 0.$$

Using the isotropy requirement and posing $A_{\mathbf{h}_j} = U_k A_{\mathbf{h}_i} U_k^\dagger$, we have

$$U_k A^\dagger_{\mathbf{h}_1} U_k^\dagger A_{\mathbf{h}_1} U_k A^\dagger_{\mathbf{h}_1} U_k^\dagger = A_{\mathbf{h}_1} U_k A^\dagger_{\mathbf{h}_1} U_k^\dagger A_{\mathbf{h}_1} = 0.$$

By exploiting Eq. (13) both the preceding equations become

$$\langle\eta_{\mathbf{h}_1}|V^\dagger_{\mathbf{h}_1}U_k^\dagger V_{\mathbf{h}_1}|\eta_{\mathbf{h}_1}\rangle\langle\eta_{\mathbf{h}_1}|U_k|\eta_{\mathbf{h}_1}\rangle = 0.$$

Then, at least one of the two following conditions must be satisfied:

$$\langle\eta_{\mathbf{h}_1}|V^\dagger_{\mathbf{h}_1}U_k^\dagger V_{\mathbf{h}_1}|\eta_{\mathbf{h}_1}\rangle = 0, \tag{17}$$

$$\langle\eta_{\mathbf{h}_1}|U_k|\eta_{\mathbf{h}_1}\rangle = 0. \tag{18}$$

Furthermore, we recall that the representation U can be chosen with unit determinant and for $s = 2$ one has $U_k = \cos\theta I + i\sin\theta\, \mathbf{n}_k \cdot \boldsymbol{\sigma}$. Then, from Eqs. (17) and (18) one has $U_k = i\mathbf{n}_k \cdot \boldsymbol{\sigma}$. Using the identity

$$U_k U_{k'} = -\mathbf{n}_k \cdot \mathbf{n}_{k'} I - i(\mathbf{n}_k \times \mathbf{n}_{k'}) \cdot \boldsymbol{\sigma}, \tag{19}$$

it follows that all the $\mathbf{n}_k$ must be mutually orthogonal and then $|K| \leqslant 4$. The case $K \cong \mathbb{Z}_3$ is not consistent with Eqs. (17) and (18). Accordingly, we end up with $K \in \{I,\mathbb{Z}_2,\mathbb{Z}_2 \times \mathbb{Z}_2,\mathbb{Z}_4\}$. Notice that, up to a change of basis, one can always choose $|\eta_{\pm\mathbf{h}_1}\rangle$ to be the eigenstates of σ_Z without loss of generality. Then, by Eqs. (17) and (18) and imposing $U_k \in \mathrm{SU}(2)\,\forall k \in K$, up to a change of basis it must be (i) $U_K := \mathrm{Rng}_K(U) = H$, where $H := \{I,i\sigma_X,i\sigma_Y,i\sigma_Z\}$ is the Heisenberg group; (ii) $U_K = J$, where $J \in \{J_i\}_{i=1}^4$, with $J_1 := \{I,i\sigma_X\}$, $J_2 := \{I,-V_{\mathbf{h}_1}(i\sigma_X)V^\dagger_{\mathbf{h}_1}\}$, $J_3 := \{I,i\sigma_X,-I,-i\sigma_X\}$, and $J_4 := \{I,-V_{\mathbf{h}_1}(i\sigma_X)V^\dagger_{\mathbf{h}_1},-I,V_{\mathbf{h}_1}(i\sigma_X)V^\dagger_{\mathbf{h}_1}\}$; or (iii) $U_K = \{I\}$. We remark that H is a projective faithful representation of $\mathbb{Z}_2 \times \mathbb{Z}_2$ in SU(2), $\{J_i\}_{i=1}^2$ are projective faithful representations of $\mathbb{Z}_2$,

[2]This is straightforward as far as $\mathbb{Z}_n$ and D_n are concerned; as for A_4 and S_4, one can verify it in a direct way considering their faithful representations given in Appendix 1 a and 1 b.

[3]We follow the argument of Ref. [27]. The condition $A^\dagger_{\mathbf{h}}A_{-\mathbf{h}} = 0$ implies that $V_{\mathbf{h}}V^\dagger_{-\mathbf{h}}$ is diagonal in the basis $\{|\eta_{+\mathbf{h}}\rangle,|\eta_{-\mathbf{h}}\rangle\}$. Since the transition matrices are not full rank, their polar decomposition is not unique: $V_{\mathbf{h}}(|\eta_{+\mathbf{h}}\rangle\langle\eta_{+\mathbf{h}}| + e^{i\theta_{\mathbf{h}}}|\eta_{-\mathbf{h}}\rangle\langle\eta_{-\mathbf{h}}|)$ gives the same polar decomposition as $V_{\mathbf{h}}\ \forall\mathbf{h} \in S$. Accordingly, one can tune the phases $\theta_{\pm\mathbf{h}}$ to choose $V_{\mathbf{h}}V^\dagger_{-\mathbf{h}} = I\ \forall\mathbf{h} \in S$.

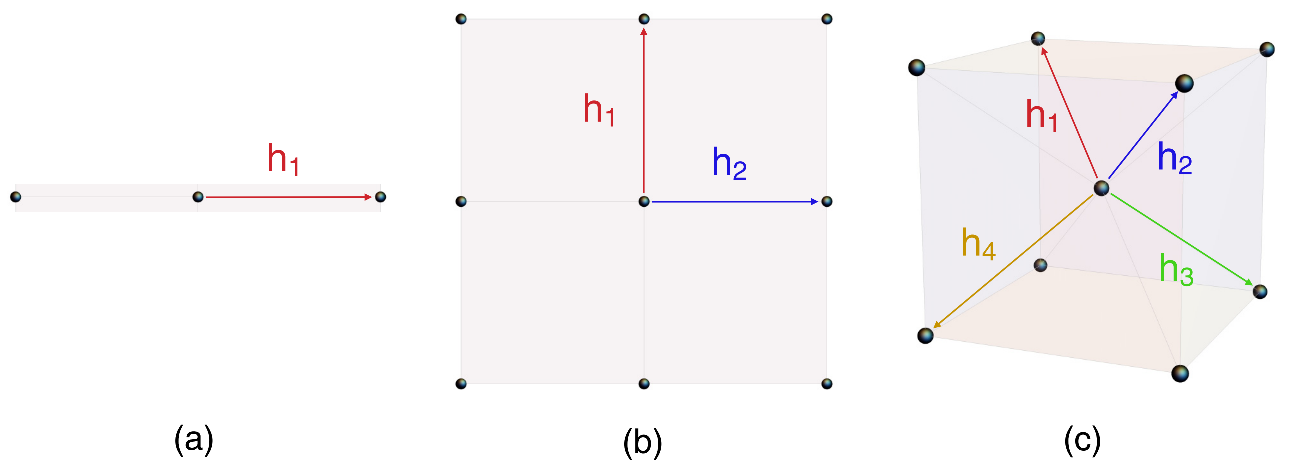

FIG. 1. Primitive cells of the unique graphs admitting isotropic QWs in dimensions $d = 1,2,3$. (a) Integer lattice. The isotropy groups can be $U_L = \{I\}$ and $U_L = \{I, i\sigma_X\}$, corresponding, respectively, to $S_+ = \{\mathbf{h}_1\}$ and $S_+ \equiv S_- = \{\mathbf{h}_1, -\mathbf{h}_1\}$. (b) Simple square lattice. The isotropy groups can be $U_L = \{I, i\sigma_X\}, \{I, i\sigma_Z\}$ and $U_L = \{I, i\sigma_X, i\sigma_Y, i\sigma_Z\}$, corresponding, respectively, to $S_+ = \{\mathbf{h}_1, \mathbf{h}_2\}$ and $S_+ \equiv S_- = \{\mathbf{h}_1, \mathbf{h}_2, -\mathbf{h}_1, -\mathbf{h}_2\}$. (c) Body-centered-cubic lattice. The only possible isotropy group is $U_L = \{I, i\sigma_X, i\sigma_Y, i\sigma_Z\}$, corresponding to $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$ with the nontrivial relator $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$. We notice that the case $d = 1$ is the only one supporting the self-interaction, namely, such that $A_e \neq 0$.

and $\{J_i\}_{i=3}^4$ are unitary faithful representations of $\mathbb{Z}_4$ in SU(2). We have thus proved the following result.

Proposition 3. If the isotropy group L contains a subgroup K such that all the $\mathbf{h}_k \in \mathcal{O}_K(\mathbf{h}_1)$ (for $\mathbf{h}_1 \in S_+$) satisfy the condition (14), then $U_K = H$, J, or I.

Isotropic QWs on $\mathbb{Z}^d$ for $d = 1,2,3$

In the Appendix we make use of Proposition 3 along with the unitarity constraints to exclude an infinite set of Cayley graphs arising from the aforementioned finite subgroups of O(3). We then proved the following.

Propostion 4. The primitive cells associated with the unique graphs admitting isotropic QWs in dimensions $d = 1,2,3$ are those shown in Fig. 1.

Throughout the present section, we solve the unitarity conditions in dimension $d = 1,2,3$ for the Cayley graphs associated with the primitive cells shown in Fig. 1 and for all the possible isotropy groups. We recall that in general each isotropy group gives rise to a distinct presentation for $\mathbb{Z}^d$, possibly with the same first-neighbor structure. As discussed in Fig. 1, different presentations can in general be associated with the same primitive cell (one can include in S_+ the inverses or not). We will now prove our main result, which is stated in Proposition 5 after the following derivation.

Before starting the derivation, we recall that in each case we can choose $|\eta_{\pm\mathbf{h}_1}\rangle$ to be the eigenstates of σ_Z. Moreover, we will make use of Eq. (13) to represent the transition matrices, recalling that $V_{\mathbf{h}} = V_{-\mathbf{h}}$. Finally, we recall that in Sec. III we showed that one can always impose the condition (9) and then multiply the transition matrices on the left by an arbitrary unitary commuting with the elements of the representation U_L.

(a) Case d = 1.

We can write the transition matrices associated with $\pm\mathbf{h}_1$ as

$$A_{\mathbf{h}_1} = \alpha_+ V|\eta_{\mathbf{h}_1}\rangle\langle\eta_{\mathbf{h}_1}|, \quad A_{-\mathbf{h}_1} = \alpha_- V|\eta_{-\mathbf{h}_1}\rangle\langle\eta_{-\mathbf{h}_1}|.$$

Multiplying the unitarity conditions on the right by $A_{\mathbf{h}_1}$ and $A^\dagger_{-\mathbf{h}_1}$, respectively,

$$\begin{aligned} A_{\mathbf{h}_1}A_e^\dagger + A_e A^\dagger_{-\mathbf{h}_1} &= 0,\\ A_e^\dagger A_{\mathbf{h}_1} + A^\dagger_{-\mathbf{h}_1} A_e &= 0, \end{aligned} \tag{20}$$

one obtains

$$A_{\pm\mathbf{h}_1}A_e^\dagger A_{\pm\mathbf{h}_1} = 0,$$

which implies that $A_e = VW$, where W has vanishing diagonal elements in the basis $\{|\eta_{+\mathbf{h}_1}\rangle, |\eta_{-\mathbf{h}_1}\rangle\}$. Substituting into Eqs. (20), one derives $\alpha_+ = \alpha_- =: n$ and, up to a change of basis, $A_e = imV\sigma_X$ with $m \geqslant 0$. Imposing the normalization condition (7) amounts to the relation $n^2 + m^2 = 1$. The admissible isotropy groups are I and, up to a change of basis, J_1. Then, for $U_L = \{I\}$, the transition matrices are given by

$$A_{\mathbf{h}_1} = V\begin{pmatrix} n & 0\\ 0 & 0\end{pmatrix}, \quad A_{-\mathbf{h}_1} = V\begin{pmatrix} 0 & 0\\ 0 & n\end{pmatrix},$$
$$A_e = V\begin{pmatrix} 0 & im\\ im & 0\end{pmatrix},$$

where V is an arbitrary unitary. For $U_L = \{I, i\sigma_X\}$, we impose the condition (9) and then V can be taken as an arbitrary unitary commuting with σ_X.

(b) Case d = 2.

The form of the transition matrices is

$$\begin{aligned} A_{\pm\mathbf{h}_1} &= \alpha_\pm V_{\mathbf{h}_1}|\eta_{\pm\mathbf{h}_1}\rangle\langle\eta_{\pm\mathbf{h}_1}|,\\ A_{\pm\mathbf{h}_2} &= \alpha_\pm V_{\mathbf{h}_2}|\eta_{\pm\mathbf{h}_2}\rangle\langle\eta_{\pm\mathbf{h}_2}|. \end{aligned}$$

Multiplying the unitarity conditions on the right by $A_{\mathbf{h}_1}$,

$$A_{\mathbf{h}_1}A^\dagger_{\pm\mathbf{h}_2} + A_{\mp\mathbf{h}_2}A^\dagger_{-\mathbf{h}_1} = 0, \tag{21}$$

one obtains

$$A_{\mathbf{h}_1}A^\dagger_{\pm\mathbf{h}_2}A_{\mathbf{h}_1} = 0.$$

The latter implies that either (i) $|\eta_{\pm\mathbf{h}_1}\rangle = |\eta_{\pm\mathbf{h}_2}\rangle$ or (ii) $|\eta_{\pm\mathbf{h}_1}\rangle = |\eta_{\mp\mathbf{h}_2}\rangle$ and that, in both cases, one can choose $V_{\mathbf{h}_1} = V_{\mathbf{h}_2}(i\sigma_Y)$ up to a change of basis. In either case, substituting into Eq. (21) one derives $\alpha_+ = \alpha_- =: \alpha$ and, from the normalization condition (7), $\alpha = \frac{1}{\sqrt{2}}$. Redefining $V := V_{\mathbf{h}_2}$, in case (i) one obtains the following family of transition matrices:

$$\begin{aligned} A_{\pm\mathbf{h}_1} &= \pm\alpha V|\eta_{\mp\mathbf{h}_1}\rangle\langle\eta_{\pm\mathbf{h}_1}|, \\ A_{\pm\mathbf{h}_2} &= \alpha V|\eta_{\pm\mathbf{h}_1}\rangle\langle\eta_{\pm\mathbf{h}_1}|. \end{aligned} \tag{22}$$

The second family, namely, case (ii), is connected to the first one via the exchange $\mathbf{h}_2 \leftrightarrow -\mathbf{h}_2$. One can check that the self-interaction term $T_e \otimes A_e$ is not supported by the unitarity conditions

$$A_{\mathbf{h}}A_e^\dagger + A_e A_{-\mathbf{h}}^\dagger = A_{\mathbf{h}}^\dagger A_e + A_e^\dagger A_{-\mathbf{h}} = 0 \quad \forall \mathbf{h} \in S,$$

namely, $A_e = 0$. Imposing Eq. (9), one can choose

$$V = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

and then multiply the transition matrices by a unitary commuting with the representation U_L. The isotropy group can be either $J_2 \equiv \{I, i\sigma_Z\}$ or H for the first family of walks, while either $J_1 = \{I, i\sigma_X\}$ or H for the second one. Thus the first family is given by

$$\begin{aligned} A_{\mathbf{h}_1} &= \frac{1}{2}V\begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \frac{1}{2}V\begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, \\ A_{\mathbf{h}_2} &= \frac{1}{2}V\begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_2} = \frac{1}{2}V\begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \end{aligned}$$

where V is either an arbitrary unitary commuting with σ_Z or $V = I$, while the second family of transition matrices is obtained exchanging $\mathbf{h}_2 \leftrightarrow -\mathbf{h}_2$ and taking V as either an arbitrary unitary commuting with σ_X or $V = I$.

(c) Case $d = 3$.

The isotropy requirement can be fulfilled with $U_L = H$. At least one of the two conditions of Eqs. (17) or (18) must be fulfilled for any nontrivial $l \in L$. Since Eq. (18) cannot be satisfied for $U_l = i\sigma_Z$, then it must be $\langle\eta_{\mathbf{h}_1}|V_{\mathbf{h}_1}^\dagger\sigma_Z V_{\mathbf{h}_1}|\eta_{\mathbf{h}_1}\rangle = 0$. This implies

$$\mathrm{Tr}\,[V_{\mathbf{h}_1}^\dagger \sigma_Z V_{\mathbf{h}_1}\sigma_Z] = 0. \tag{23}$$

Writing $V_{\mathbf{h}_1}$ in the general unitary form

$$V_{\mathbf{h}_1} = \theta\begin{pmatrix} \mu & -\nu^* \\ \nu & \mu^* \end{pmatrix},$$

where $|\theta|^2 = |\mu|^2 + |\nu|^2 = 1$, the condition in Eq. (23) implies that $|\mu| = |\nu| = 2^{-1/2}$, and using the polar decomposition (13) of $A_{\pm\mathbf{h}_1}$ we obtain

$$A_{\mathbf{h}_1} = \frac{\alpha_+}{\sqrt{2}}\begin{pmatrix} \phi & 0 \\ \psi & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \frac{\alpha_-}{\sqrt{2}}\begin{pmatrix} 0 & -\psi^* \\ 0 & \phi^* \end{pmatrix}, \tag{24}$$

with ϕ and ψ phase factors. Using isotropy, namely, considering the orbit of the above matrices under conjugation with H, we obtain

$$\begin{aligned} A_{\mathbf{h}_2} &= \frac{\alpha_+}{\sqrt{2}}\begin{pmatrix} 0 & \psi \\ 0 & \phi \end{pmatrix}, \quad A_{-\mathbf{h}_2} = \frac{\alpha_-}{\sqrt{2}}\begin{pmatrix} \phi^* & 0 \\ -\psi^* & 0 \end{pmatrix}, \\ A_{\mathbf{h}_3} &= \frac{\alpha_+}{\sqrt{2}}\begin{pmatrix} 0 & -\psi \\ 0 & \phi \end{pmatrix}, \quad A_{-\mathbf{h}_3} = \frac{\alpha_-}{\sqrt{2}}\begin{pmatrix} \phi^* & 0 \\ \psi^* & 0 \end{pmatrix}, \\ A_{\mathbf{h}_4} &= \frac{\alpha_+}{\sqrt{2}}\begin{pmatrix} \phi & 0 \\ -\psi & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_4} = \frac{\alpha_-}{\sqrt{2}}\begin{pmatrix} 0 & \psi^* \\ 0 & \phi^* \end{pmatrix}. \end{aligned} \tag{25}$$

Also in this case, the self-interaction term is not supported by the unitarity conditions. Finally, we can write the matrix $A_{\mathbf{k}}$ in Eq. (6) as

$$A_{\mathbf{k}} = \sum_{i=1}^{4}(A_{\mathbf{h}_i}e^{ik_i} + A_{-\mathbf{h}_i}e^{-ik_i})$$

and imposing unitarity of $A_{\mathbf{k}}$ for every $\mathbf{k}$ we obtain the conditions

$$\alpha_+^2 = \alpha_-^2 = \tfrac{1}{4}, \quad \phi^{*2} + \phi^2 = \psi^{*2} + \psi^2 = 0,$$

namely,

$$\phi,\psi \in \left\{\pm\zeta^+ := \pm\frac{1+i}{\sqrt{2}}, \pm\zeta^- := \pm\frac{1-i}{\sqrt{2}}\right\}.$$

The different choices of the overall signs for ϕ and ψ are connected to each other by an overall phase factor and by unitary conjugation by σ_Z. Then we can fix them by choosing the plus signs. The choices $\phi = \zeta^\pm$ and $\psi = \zeta^\mp$ are equivalent to $\phi = \psi = \zeta^\pm$ via conjugation of the former by $e^{\pm i(\pi/4)\sigma_Z}$ and an exchange $\mathbf{h}_1 \leftrightarrow \mathbf{h}_4$. Accordingly, the QWs found are given by the transition matrices of Eqs. (24) and (25) with $\psi = \varphi = \zeta^\pm$, namely, the two Weyl QWs presented in Ref. [9].

We have thus proved the following main result.

Proposition 5 (classification of the isotropic QWs on lattices of dimension $d = 1,2,3$ *with a coin system of dimension* $s = 2$*).* Let $S = S_+ \cup S_- \cup \{e\}$ denote a set of generators for $\mathbb{Z}^d$ and let $\{A_{\mathbf{h}}\}_{\mathbf{h}\in S}$ denote the set of transition matrices of a QW on $\mathbb{Z}^d$ with a coin system of dimension $s = 2$ and isotropic on S_+. Then for each $d = 1,2,3$ the admissible graphs are unique (see Fig. 1) and one has the following. (a) For case $d = 1$ one has

$$\begin{aligned} A_{\mathbf{h}_1} &= V\begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = V\begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix}, \\ A_e &= V\begin{pmatrix} 0 & im \\ im & 0 \end{pmatrix}, \end{aligned}$$

where n and m are real such that $n^2 + m^2 = 1$, and V is an arbitrary unitary if $S_+ = \{\mathbf{h}_1\}$ or V is a unitary commuting with σ_X if $S_+ = \{\mathbf{h}_1, -\mathbf{h}_1\}$. (b) For case $d = 2$ one has $A_e = 0$ and

$$\begin{aligned} A_{\mathbf{h}_1} &= \frac{1}{2}V\begin{pmatrix} 1 & 0 \\ 1 & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \frac{1}{2}V\begin{pmatrix} 0 & -1 \\ 0 & 1 \end{pmatrix}, \\ A_{\mathbf{h}_2} &= \frac{1}{2}V\begin{pmatrix} 0 & 1 \\ 0 & 1 \end{pmatrix}, \quad A_{-\mathbf{h}_2} = \frac{1}{2}V\begin{pmatrix} 1 & 0 \\ -1 & 0 \end{pmatrix}, \end{aligned}$$

where V is a unitary commuting with σ_X if $S_+ = \{\mathbf{h}_1, \mathbf{h}_2\}$ or $V = I$ if $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, -\mathbf{h}_1, -\mathbf{h}_2\}$. (c) For case $d = 3$ one has $A_e = 0$ and

$$A_{\mathbf{h}_1} = \begin{pmatrix} \eta^{\pm} & 0 \\ \eta^{\pm} & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_1} = \begin{pmatrix} 0 & -\eta^{\mp} \\ 0 & \eta^{\mp} \end{pmatrix},$$

$$A_{\mathbf{h}_2} = \begin{pmatrix} 0 & \eta^{\pm} \\ 0 & \eta^{\pm} \end{pmatrix}, \quad A_{-\mathbf{h}_2} = \begin{pmatrix} \eta^{\mp} & 0 \\ -\eta^{\mp} & 0 \end{pmatrix},$$

$$A_{\mathbf{h}_3} = \begin{pmatrix} 0 & -\eta^{\pm} \\ 0 & \eta^{\pm} \end{pmatrix}, \quad A_{-\mathbf{h}_3} = \begin{pmatrix} \eta^{\mp} & 0 \\ \eta^{\mp} & 0 \end{pmatrix},$$

$$A_{\mathbf{h}_4} = \begin{pmatrix} \eta^{\pm} & 0 \\ -\eta^{\pm} & 0 \end{pmatrix}, \quad A_{-\mathbf{h}_4} = \begin{pmatrix} 0 & \eta^{\mp} \\ 0 & \eta^{\mp} \end{pmatrix},$$

where $\eta^{\pm} = \frac{1 \pm i}{4}$ and $S_+ = \{\mathbf{h}_1, \mathbf{h}_2, \mathbf{h}_3, \mathbf{h}_4\}$ with the nontrivial relator $\mathbf{h}_1 + \mathbf{h}_2 + \mathbf{h}_3 + \mathbf{h}_4 = 0$.

VI. CONCLUSION

In this paper we presented a complete classification of the isotropic quantum walks on lattices of dimension $d = 1,2,3$ with coin dimension $s = 2$. We have extended the isotropy definition of Ref. [9] to account for groups with generators of different orders. We introduced a technique to construct the Cayley graphs of a given group G satisfying a relevant necessary condition for isotropy. This allowed us to exclude an infinite class of Cayley graphs of $\mathbb{Z}^d$. The technique is sufficiently flexible to be used in the future for other generally non-Abelian groups. Remarkably, the Cayley graph is unique for each dimension $d = 1,2,3$ and for $d = 3$ the only admissible QWs are the two Weyl QWs presented in Ref. [9]. The use of isotropy since the very beginning has made the solution of the unitarity equations significantly shorter. Moreover, we eliminated the superfluous technical assumption used in Ref. [9] and mentioned in the Introduction. In consideration of the length of the derivation from informational principles of the Weyl equation in Ref. [9], the present derivation constitutes a thoroughly independent check. Finally, this result represents an extension of the classification of Ref. [24].

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APPENDIX: EXCLUDING CAYLEY GRAPHS

In Appendix 1–4 we will exclude the infinite family of graphs arising from the following finite isotropy groups $L <$ O(3): (1) A_4, S_4, and their direct product with $\mathbb{Z}_2$ (except for the cases in item 2); (2) the special instances of item 1 where the orbits contain the vertices of a truncated tetrahedron; (3) $\mathbb{Z}_n$ and D_n for $n = 3,4,6$ and their direct product with $\mathbb{Z}_2$; and (4) one special instance arising from D_2, $D_2 \times \mathbb{Z}_2$.

1. Excluding A_4- and S_4-symmetric Cayley graphs

In this section we use the convention that unwritten matrix elements are zero. In Secs. 1 a and 1 b we will consider the orbit of an arbitrary three-dimensional vector $\mathbf{v} = (\alpha,\beta,\gamma)^T$ under the action of the finite groups $L \cong A_4, S_4$ in O(3). To this purpose, as discussed in Sec. IV, we will use the real, orthogonal, and three-dimensional faithful representations of L, identifying its representation with the group itself. In the present case of $L \cong A_4, S_4$, such representations coincide with the irreducible ones, since the reducible ones cannot be faithful [otherwise they would have orthogonal blocks of dimension at most 2, but A_4, S_4 are not subgroups of O(2)].

We denote by $\mathcal{O}_L(\mathbf{v})$ the family of orbits of $\mathbf{v}$ under the action of L, parametrized by α,β,γ. Each orbit satisfies a necessary condition to give rise to an isotropic presentation for $\mathbb{Z}^d$ for $d = 1,2,3$.

Proposition 6. If L contains a ternary subgroup $K \cong \mathbb{Z}_3$ such that for $\mathbf{h}_i, \mathbf{h}_j \in \mathcal{O}_K(\mathbf{v})$ and $\mathbf{h}_l, \mathbf{h}_m \in \mathcal{O}_L(\mathbf{v})$ the condition in Eq. (14) is satisfied, then the set of vertices $\mathcal{O}_L(\mathbf{v})$ cannot satisfy the necessary conditions (16) and (15) for unitarity.

Proof. By Proposition 3, K has to be a subgroup of the Heisenberg group H. However, H does not contain ternary subgroups. ■

We will make use of Proposition 6 to exclude an infinite family of presentations arising from $L \cong A_4, S_4$. Since by Eq. (14) we are interested in sums or differences of generators, the cases $L \cong A_4 \times \mathbb{Z}_2, S_4 \times \mathbb{Z}_2$ are already accounted for: Their irreducible representations just add the inversion to the irreducible ones of A_4, S_4.

The groups L contain four isomorphic copies of $\mathbb{Z}_3$ (see Secs. 1 a and 1 b). Let us denote by D the generator of one of these cyclic subgroups. The content of Eq. (14) for a fixed choice of i,j translates to the following. Suppose that for all $A,B \in L_0 := \{0 \in M_3(\mathbb{R})\} \cup L$ one has

$$(I - D)\mathbf{v} = s(A + tB)\mathbf{v} \Leftrightarrow (sA\mathbf{v} = \mathbf{v}) \vee (stB\mathbf{v} = \mathbf{v}) \quad \text{(A1)}$$

(s,t signs). Our strategy is now to solve the necessary conditions for the violation of (A1), consisting in systems of the form

$$(I - D - s(A + tB))\mathbf{v} = 0 \quad \forall A,B \in L_0. \quad \text{(A2)}$$

These will produce some solutions $\mathbf{v}_0$. Then we can choose another vector in $\mathcal{O}_L(\mathbf{v}_0)$, impose again Eq. (A2), and iterate until we end up either with the trivial solution or with a system of linear equations for α,β,γ. By Proposition 6, the only A_4- or S_4-symmetric Cayley graphs of $\mathbb{Z}^3$ for which the unitarity conditions may be satisfied must then be found among the nontrivial solutions of the above systems. Since only the condition (A2) is necessary, we need to check whether the solutions actually violate the condition (A1). The remaining differences $(D - D^2)\mathbf{v}$ and $(D^2 - I)\mathbf{v}$ are the orbit of $(I - D)\mathbf{v}$ under D; then we can just solve (A2) and check (A1).

In the following we will show that (A1) has only trivial solutions for $A,B \in L$, except for the special case where $\mathbf{v} = \alpha(3,1,1)^T$, which will be treated separately in Sec. 2. At the end of Sec. 1 b we will then prove the same result in the case of $B = 0$.

It is useful to notice the following.

Remark 1. $\mathbf{v}_1 \in \mathbb{R}^3$ solves

$$[I - D - s(A + tB)]\mathbf{v}_1 = 0$$

if and only if $\mathbf{v}_2 := F_2^{-1}\mathbf{v}_1$ solves

$$F_1[I - D - s(A + tB)]F_2\mathbf{v}_2 = 0$$

for some arbitrary $F_1, F_2 \in \mathrm{GL}(3,\mathbb{R})$. In particular, this is relevant in the case $F_2 \in L$, because it means that the orbits generated by the two solutions $\mathbf{v}_1$ and $\mathbf{v}_2$ coincide.

This remark will allow us to considerably reduce the number of systems we have to solve. In the following we will refer to a particular solution for (A2) indifferently with (i) the solution vector $\mathbf{v}_0$, (ii) the lattice which $\mathbf{v}_0$ gives rise to, (iii) the polyhedron whose vertices are the elements of $\mathcal{O}_L(\mathbf{v}_0)$, (iv) any other vector in $\mathcal{O}_L(\mathbf{v}_0)$, or (v) the orbit $\mathcal{O}_L(\mathbf{v}_0)$. The cases we will end up with are the following:

(1) The simple cubic lattice, generated orbiting $\mathbf{v}_s = \alpha(1,0,0)^T$ under A_4, has its vertices all signed permutations of the coordinates of $\mathbf{v}_s$.

(2) The bcc lattice, generated orbiting $\mathbf{v}_b = \alpha(1,-1,-1)^T$ under S_4, has its vertices all signed permutations of the coordinates of $\mathbf{v}_b$.

(3) The cuboctahedron has vertices that are all signed permutations of the coordinates of $\mathbf{v}_c = \alpha(1,-1,0)^T$ and are generated by orbiting $\mathbf{v}_c$ under A_4.

(4) The truncated tetrahedron has vertices that are all permutations with an even number of minus signs of the coordinates of $\mathbf{v}_{tt} = \alpha(3,1,1)^T$ and are generated by orbiting $\mathbf{v}_{tt}$ under A_4; in addition, one can also find the solution including the inverses, which is given by $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$.

(5) The truncated octahedron has vertices that are all signed permutations of the coordinates of $\mathbf{v}_{to} = \alpha(1,-2,0)^T$ and are generated by orbiting $\mathbf{v}_{to}$ under S_4.

One can easily check that $\mathcal{O}_L(\mathbf{v}_0)$ for the five cases above actually are generating sets for some presentation of $\mathbb{Z}^3$.

In the following, we will choose $D = R$ with $R(x,y,z)^T = (z,x,y)^T$ (R is contained in the representation of both A_4 and S_4). As a consequence, we can consider $A \neq B$, since otherwise there are two possible cases. The first is $(I - R)\mathbf{v} = \pm 2A\mathbf{v}$, implying that $(A^{-1} - A^{-1}R)\mathbf{v} = \pm 2\mathbf{v}$. Since $A, R \in \mathrm{O}(3)$, by the triangle inequality it must be

$$A^{-1}\mathbf{v} = \pm\mathbf{v},\ A^{-1}R\mathbf{v} = \mp\mathbf{v},$$

and in particular $\mathbf{v} = -R\mathbf{v}$ holds. This implies that $\mathbf{v} = (0,0,0)^T$. The second is $(I - R)\mathbf{v} = 0$, implying that $\mathbf{v} = \alpha(1,1,1)^T$.

Finally, the reader can check that for $\mathbf{v}_0 \in \{\mathbf{v}_s, \mathbf{v}_b, \mathbf{v}_c, \mathbf{v}_{to}\}$ the condition (A1) is not violated, thus excluding the cases of $S_+ = \mathcal{O}_L(\mathbf{v}_0)$ by virtue of Proposition 6.

a. Excluding A_4-symmetric Cayley graphs

A_4 has a unique three-dimensional real irreducible representation, generated by the matrices

$$X_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad R = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}. \qquad \text{(A3)}$$

We define

$$X_0 = I, \quad X_2 = RX_1R^{-1}, \quad X_3 = R^2X_1R^{-2}.$$

The group contains four isomorphic copies of $\mathbb{Z}_3$, generated, respectively, by the elements of the set $\{R, X_1R, X_2R, X_3R\}$ (these are cyclic signed permutations of the coordinates).

We now choose the subgroup generated by R and consider the difference $(I - R)\mathbf{v}$, setting the condition (A2) for any $A, B \in A_4$. Each of these define linear systems of three equations for $\mathbf{v}$. If A equals I or R, then it is easy to see that $\exists G \in A_4$ such that $G\mathbf{v} = s\mathbf{v}$ (s a sign): This implies that either $\mathbf{v} = (0,\beta,\gamma)^T$ up to signed permutations or $\mathcal{O}_{A_4}(\mathbf{v}) = \mathcal{O}_{A_4}(\mathbf{v}_b)$. The latter case was excluded in Sec. 1. The remaining cases are then (i) $A, B \notin \{I, R\}$ or (ii) $\mathbf{v} = (0,\beta,\gamma)^T$ and signed permutations. Case (ii), however, will appear as a special instance of (i). In case (i), we have six cases for $s(A + tB)$: (1) $s(X_i + tX_j) = \begin{pmatrix} 2s & & \\ & \pm\xi & \\ & & 0 \end{pmatrix}$, modulo permutations of the diagonal elements, with arbitrary sign s and for $\xi := 0,2$; (2) $s(X_i + tX_jR) = \begin{pmatrix} s_1 & 0 & t_1 \\ t_2 & s_2 & 0 \\ 0 & t_3 & s_3 \end{pmatrix}$, with $s_1s_2 + s_1s_3 + s_2s_3 = t_1t_2 + t_1t_3 + t_2t_3 = -1$; (3) $s(X_i + tX_jR^2) = \begin{pmatrix} s_1 & t_1 & 0 \\ 0 & s_2 & t_2 \\ t_3 & 0 & s_3 \end{pmatrix}$, with arbitrary signs t_k, and $s_1s_2 + s_1s_3 + s_2s_3 = -1$; (4) $s(X_i + tX_j)R = \begin{pmatrix} & & 2s \\ \pm\xi & & \\ & 0 & \end{pmatrix}$ and permutations of the written elements, with arbitrary sign s and $\xi = 0,2$; (5) $s(X_i + tX_jR)R = \begin{pmatrix} 0 & t_1 & s_1 \\ s_2 & 0 & t_2 \\ t_3 & s_3 & 0 \end{pmatrix}$, with arbitrary signs t_k, and $s_1s_2 + s_1s_3 + s_2s_3 = -1$; and (6) $s(X_i + tX_j)R^2 = \begin{pmatrix} & 2s & \\ & & \pm\xi \\ 0 & & \end{pmatrix}$ and permutations of the written elements, with arbitrary sign s and $\xi = 0,2$.

All the above-mentioned permutations of elements and those between the s_i and t_i are performed by conjugation with $R^{\pm 1}$. Since

$$[I - R - sR(A + tB)R^{-1}] = R[I - R - s(A + tB)]R^{-1},$$

by Remark 1 we can just choose one permutation in each of the six cases to find the orbits of the solutions.

Accordingly, explicitly computing the expression

$$I - R - s(A + tB) = \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix} - s(A + tB),$$

we end up with the following cases: (1) $\begin{pmatrix} 1+2s & 0 & -1 \\ -1 & 1\pm\xi & 0 \\ 0 & -1 & 1 \end{pmatrix}$ for s arbitrary sign; (2) $\begin{pmatrix} 2 & & -2 \\ -\xi' & \xi & \\ & 0 & 0 \end{pmatrix}$, $\begin{pmatrix} 2 & & 0 \\ -2 & \xi & \\ & -\xi' & 0 \end{pmatrix}$, and $\begin{pmatrix} 0 & & -2 \\ -\xi' & 2 & \\ & 0 & \xi \end{pmatrix}$, with $\xi, \xi' = 0,2$; (3) $\begin{pmatrix} 2 & s_1 & -1 \\ -1 & \xi & s_2 \\ s_3 & -1 & 0 \end{pmatrix}$, with s_i arbitrary; (4) $\begin{pmatrix} 1 & 0 & 2s-1 \\ -1 & 1 & 0 \\ 0 & \pm\xi - 1 & 1 \end{pmatrix}$, with s arbitrary; (5) $\begin{pmatrix} 1 & s_1 & 0 \\ -2 & 1 & s_2 \\ s_3 & -\xi & 1 \end{pmatrix}$, with s arbitrary; and (6) $\begin{pmatrix} 1 & 2s & -1 \\ -1 & 1 & 0 \\ \pm\xi & -1 & 1 \end{pmatrix}$, with s arbitrary. The only solution to cases 1 and 4 is $\mathcal{O}_{A_4}(\mathbf{v}_b)$. Cases 3, 5, and 6 can be treated together since they exhibit a common structure: Their solutions are $\mathcal{O}_{A_4}(\mathbf{v}_b)$ (which has been already excluded by Proposition 6) and $\mathcal{O}_{A_4}(\mathbf{v}_{tt})$ (which is excluded in Sec. 2). The only relevant case is 2, since all the other cases have been already excluded.

In case 2, the most general orbits of solutions are $\mathcal{O}_{A_4}(\mathbf{v}_i)$ for $i = 1,2,3$, where

$$\mathbf{v}_1 = \begin{pmatrix} \alpha \\ \beta \\ \alpha \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 0 \\ \beta \\ \gamma \end{pmatrix}, \quad \mathbf{v}_3 = R^2\mathbf{v}_2. \tag{A4}$$

Nevertheless, for $\mathbf{v} \in \{\mathbf{v}_2,\mathbf{v}_3\}$ the condition (A1) is not violated. Indeed, $\mathbf{v}_2$ was found as a solution of

$$(I - R + X_1 - RX_1)\mathbf{v}_2 = 0; \tag{A5}$$

however, $X_1\mathbf{v}_2 = -\mathbf{v}_2$ and thus Eq. (A1) is satisfied. A similar argument holds for $\mathbf{v}_3$. By virtue of Proposition 6 the corresponding orbits $\mathcal{O}_{A_4}(\mathbf{v}_2)$ and $\mathcal{O}_{A_4}(\mathbf{v}_3)$ are excluded.

From the above analysis we already know that the only relevant solution is $\mathbf{v}_1$ for case 2, modulo cyclic permutations. We now impose that $X_1\mathbf{v}_1$, which is in $\mathcal{O}_{A_4}(\mathbf{v}_1)$, is itself a solution of Eq. (A2). Thus we impose

$$X_1\mathbf{v}_1 = \mathbf{w} \in \left\{ \begin{pmatrix} \alpha' \\ \beta' \\ \alpha' \end{pmatrix}, \begin{pmatrix} \alpha' \\ \alpha' \\ \beta' \end{pmatrix}, \begin{pmatrix} \beta' \\ \alpha' \\ \alpha' \end{pmatrix} \right\}.$$

The solutions are $\mathcal{O}_{A_4}(\mathbf{v}_s)$ and $\mathcal{O}_{A_4}(\mathbf{v}_b)$: We can exclude also this last case.

b. Excluding S_4-symmetric Cayley graphs

The group S_4 contains A_4 as a subgroup of index 2. The element connecting the two cosets is an involution, which we will denote by C. The group S_4 has two three-dimensional irreducible representations: Their elements are signed permutation matrices of three elements and the two representations coincide up to a minus sign on the elements in the coset CA_4. Nevertheless, in our case the sign is irrelevant, since we are considering combinations $s(A + tB)$ of $A,B \in S_4$ with s,t arbitrary signs. Accordingly, we consider the representation resulting from orbiting the elements generated by (A3) under the left action of $\{I,C\}$ with

$$C = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix},$$

whose effect is just an exchange of the first and third rows.

Let us now define $X_i' := CX_i$. In order to perform the computation of $s(A + tB)$, we proceed as follows. We have to compute

$$\begin{gathered} s(X_i + tX_j), \quad s(X_i' + tX_j'), \\ s(X_i + tX_jR), \quad s(X_i' + tX_j'R), \\ s(X_i' + tX_j), \quad s(X_i' + tX_jR), \quad s(X_i' + tX_jR^2) \end{gathered} \tag{A6}$$

and then recover all the remaining combinations by right multiplication of these by $R^{\pm 1}$. For (A6), we obtain the following cases: (1) $\begin{pmatrix} \pm 2 & & \\ & \xi & \\ & & 0 \end{pmatrix}$ and $\begin{pmatrix} & & \pm 2 \\ & \xi & \\ 0 & & \end{pmatrix}$, considering all the permutations of elements and $\xi = 0, \pm 2$, and (2) $\begin{pmatrix} s_1 & & t_1 \\ t_2 & s_2 & \\ & t_3 & s_3 \end{pmatrix}$, $\begin{pmatrix} & t_1 & s_1 \\ t_2 & s_2 & \\ s_3 & & t_3 \end{pmatrix}$, $\begin{pmatrix} s_1 & & s_2 \\ & \xi & \\ s_3 & & s_4 \end{pmatrix}$, $\begin{pmatrix} & & \xi \\ t_2 & s_2 & \\ s_3 & t_3 & \end{pmatrix}$, and $\begin{pmatrix} & t_1 & s_1 \\ & s_2 & t_2 \\ \xi & & \end{pmatrix}$ for $\xi = 0, \pm 2$. As mentioned above, one has to add to these cases the matrices resulting from a right multiplication of the previous ones by $R^{\pm 1}$, whose action is a cyclic permutation of the columns. Let us now consider

$$I - R = \begin{pmatrix} 1 & 0 & -1 \\ -1 & 1 & 0 \\ 0 & -1 & 1 \end{pmatrix}$$

and derive the matrices

$$I - R + s(A + tB)R^i, \quad i = 0, \pm 1 \tag{A7}$$

for all the mentioned cases: (1) It is easy to verify that, in this case, either the matrices in Eq. (A7) have a trivial solution or their solutions are $\mathcal{O}_{S_4}(\mathbf{v}_b)$ (already excluded) and $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$ (which will be treated in Sec. 2) and (2)

$$\begin{pmatrix} 1+s_1 & & t_1-1 \\ t_2-1 & 1+s_2 & \\ & t_3-1 & 1+s_3 \end{pmatrix}, \quad \begin{pmatrix} 1 & & \xi-1 \\ t_2-1 & 1+s_2 & \\ s_3 & t_3-1 & 1 \end{pmatrix},$$

$$\begin{pmatrix} 1 & t_1 & s_1-1 \\ s_2-1 & 1 & t_2 \\ t_3 & s_3-1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & \xi & -1 \\ s_2-1 & 1 & t_2 \\ t_3 & -1 & 1+s_3 \end{pmatrix},$$

$$\begin{pmatrix} 1+t_1 & s_1 & -1 \\ -1 & 1+t_2 & s_2 \\ s_3 & -1 & 1+t_3 \end{pmatrix}, \quad \begin{pmatrix} 1+\xi & & -1 \\ -1 & 1+t_2 & s_2 \\ & s_3-1 & 1+t_3 \end{pmatrix},$$

$$\begin{pmatrix} 1 & t_1 & s_1-1 \\ t_2-1 & 1+s_2 & \\ s_3 & -1 & 1+t_3 \end{pmatrix}, \quad \begin{pmatrix} 1+t_1 & s_1 & -1 \\ s_2-1 & 1+t_2 & \\ & -1 & \xi+1 \end{pmatrix},$$

$$\begin{pmatrix} 1+t_1 & s_1 & -1 \\ s_2-1 & 1 & t_2 \\ & t_3-1 & 1+s_3 \end{pmatrix}, \quad \begin{pmatrix} 1+s_1 & & t_1-1 \\ t_2-1 & 1 & s_2 \\ & \xi-1 & 1 \end{pmatrix},$$

$$\begin{pmatrix} 1+s_1 & & t_1-1 \\ -1 & 1+t_2 & s_2 \\ t_3 & s_3-1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 1 & t_1 & s_1-1 \\ -1 & 1+s_2 & t_2 \\ \xi & -1 & 1 \end{pmatrix},$$

$$\begin{pmatrix} 1+s_1 & & s_2-1 \\ -1 & 1+\xi & \\ s_3 & -1 & 1+s_4 \end{pmatrix}, \quad \begin{pmatrix} 1 & s_2 & s_1-1 \\ \xi-1 & 1 & \\ & s_4-1 & 1+s_3 \end{pmatrix},$$

$$\begin{pmatrix} 1+s_2 & s_1 & -1 \\ -1 & 1 & \xi \\ s_4 & s_3-1 & 1 \end{pmatrix}.$$

The above set can be partitioned into equivalence classes according to the relation

$$N \sim M \Leftrightarrow \exists F \in S_4, \quad F' \in \mathrm{GL}(3,\mathbb{R}) \,:\, N = F'MF. \tag{A8}$$

By Remark 1 the above equivalence relation preserves the orbits of solutions of the linear systems. It is easy to check that there are five equivalence classes represented by the following matrices:

$$M_1 = \begin{pmatrix} 1+s_1 & & s_2-1 \\ -1 & 1+\xi & \\ s_3 & -1 & 1+s_4 \end{pmatrix},$$

$$M_2 = \begin{pmatrix} 1+s_1 & & t_1-1 \\ t_2-1 & 1+s_2 & \\ & t_3-1 & 1+s_3 \end{pmatrix},$$

$$M_3 = \begin{pmatrix} 1 & t_1 & s_1-1 \\ t_2-1 & 1+s_2 & \\ s_3 & -1 & 1+t_3 \end{pmatrix},$$

$$M_4 = \begin{pmatrix} 1 & t_1 & s_1-1 \\ s_2-1 & 1 & t_2 \\ t_3 & s_3-1 & 1 \end{pmatrix},$$

$$M_5 = \begin{pmatrix} 1 & \xi & -1 \\ s_2-1 & 1 & t_2 \\ t_3 & -1 & 1+s_3 \end{pmatrix}.$$

The solutions for M_4 and M_5 are $\mathcal{O}_{S_4}(\mathbf{v}_s)$, $\mathcal{O}_{S_4}(\mathbf{v}_b)$ (which have been already excluded), and $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$, which will be treated in Sec. 2.

The three remaining cases are given in the following. (1) For M_1 one has $\mathcal{O}_{S_4}(\mathbf{v}_s)$, $\mathcal{O}_{S_4}(\mathbf{v}_b)$, $\mathcal{O}_{S_4}(\mathbf{v}_c)$, $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$, $\mathcal{O}_{S_4}(\mathbf{v}_1)$, and $\mathcal{O}_{S_4}(\mathbf{v}_2)$, with

$$\mathbf{v}_1 = \begin{pmatrix} \alpha \\ \alpha \\ \beta \end{pmatrix}, \quad \mathbf{v}_2 = \alpha \begin{pmatrix} 3 \\ 1 \\ 2 \end{pmatrix}.$$

The systems in the same equivalence class are connected by the permutations $F \in \{R^{\pm 1}, C, CR^{\pm 1}\}$. (2) For M_2 one has $\mathcal{O}_{S_4}(\mathbf{v}_1)$ and $\mathcal{O}_{S_4}(\mathbf{v}_3)$, with

$$\mathbf{v}_3 = \begin{pmatrix} 0 \\ \alpha \\ \beta \end{pmatrix}.$$

(3) For M_3 one has $\mathcal{O}_{S_4}(\mathbf{v}_s)$, $\mathcal{O}_{S_4}(\mathbf{v}_b)$, $\mathcal{O}_{S_4}(\mathbf{v}_c)$, $\mathcal{O}_{S_4}(\mathbf{v}_t o)$, $\mathcal{O}_{S_4}(\mathbf{v}_1)$, and $\mathcal{O}_{S_4}(\mathbf{v}_4)$, with

$$\mathbf{v}_4 = \begin{pmatrix} \alpha \\ \beta \\ \frac{\alpha+\beta}{2} \end{pmatrix}.$$

The systems in the same equivalence class are connected by the permutations $F \in \{R^2, C\}$.

We notice that $\mathbf{v}_2$ is a particular case of $\mathbf{v}_4$; then we can just treat the latter. On the other hand, the vectors in $\mathcal{O}_{S_4}(\mathbf{v}_3)$ cannot be solutions for M_i with $i \neq 2$; otherwise the orbit is reduced to $\mathcal{O}_{S_4}(\mathbf{v}_s)$, $\mathcal{O}_{S_4}(\mathbf{v}_c)$, or $\mathcal{O}_{S_4}(\mathbf{v}_{to})$, which are ruled out. The remaining case of $\mathcal{O}_{S_4}(\mathbf{v}_3)$ can then be excluded via the same analysis of case 2 in the previous section.

We end up with $\mathcal{O}_{S_4}(\mathbf{v}_1)$ and $\mathcal{O}_{S_4}(\mathbf{v}_4)$. We observe that imposing that $X_2\mathbf{v}_1$ is a solution for M_1, M_2, and M_3 gives rise to $\mathcal{O}_{S_4}(\mathbf{v}_s)$, $\mathcal{O}_{S_4}(\mathbf{v}_b)$, and $\mathcal{O}_{S_4}(\mathbf{v}_c)$. As for $\mathcal{O}_{S_4}(\mathbf{v}_4)$, imposing that $X_2\mathbf{v}_4$ is a solution leads to $\mathcal{O}_{S_4}(\mathbf{v}_{tt})$, $\mathcal{O}_{S_4}(\mathbf{v}_{to})$, and $\mathcal{O}_{S_4}(\mathbf{v}_5)$ with $\mathbf{v}_5 = \alpha(5,3,1)^T$. However, it is easy to verify that $(I - X_2R)\mathbf{v}_5$ is uniquely determined as the sum of elements of $\{\mathbf{0}, \mathcal{O}_{S_4}(\pm\mathbf{v}_5)\}$, leading us to exclude this last case by virtue of Proposition 6. Finally, as anticipated at the beginning of Sec. 1, we can exclude $(I - R)\mathbf{v} = \pm A\mathbf{v}$ for $A \in L$ and $L \cong A_4, S_4$: By direct inspection of the representation matrices of S_4, it turns out that this condition leads to $\mathcal{O}_{S_4}(\mathbf{v}_c)$.

2. Exclusion of the truncated tetrahedron

In this section we make use of the three-dimensional irreducible representation of A_4 provided in Sec. 1 a in order to exclude, by means of the unitarity conditions, the graph whose primitive cell is the set of vertices of the truncated tetrahedron. This also excludes the case where the inverses are contained in S_+. For notational convenience, we will use the Pauli matrix notation $X := X_1$, $Y := X_2$, and $Z := X_3$ and use the vector $\mathbf{w}_{tt} = \alpha(1,1,3)^T$ instead of $\mathbf{v}_{tt}$ as a representative of the orbit $\mathcal{O}_{A_4}(\mathbf{v}_{tt})$. In the following we will also denote the elements $G\mathbf{w}_{tt}$ (for $G \in A_4$) by the shorthand G.

Let U be a faithful unitary and (generally projective) representation of A_4 in SU(2). We will define the transition matrices as

$$A_{\pm G} := U_G A_{\pm I} U_G^\dagger, \tag{A9}$$

with $G \in A_4$. From the unitarity conditions (8), choosing $\mathbf{h}'' = 2\mathbf{w}_{tt}$, one derives the form

$$A_{\pm I} := \alpha_\pm V|\pm\rangle\langle\pm|, \tag{A10}$$

with $\{|+\rangle, |-\rangle\}$ the orthonormal basis, $\alpha_\pm > 0$, and V unitary. Consider the following unitarity conditions:

$$A_I A_W^\dagger + A_{-W} A_{-I}^\dagger = 0, \quad W = X, Y.$$

By multiplication on the right by A_I we obtain

$$A_I A_W^\dagger A_I = 0,$$

implying that U_W must be antidiagonal in the $\{|+\rangle, |-\rangle\}$ basis or in $\{V|+\rangle, V|-\rangle\}$. On the other hand, from

$$A_I A_{-R}^\dagger + A_R A_{-I}^\dagger = 0$$

one gets

$$A_{-I} A_R^\dagger A_{-I} = 0, \tag{A11}$$

meaning that U_R must be diagonal in $\{|+\rangle, |-\rangle\}$ or $\{V|+\rangle, V|-\rangle\}$.

Let us now suppose that U_X is antidiagonal in $\{|+\rangle, |-\rangle\}$ and U_Y antidiagonal in $\{V|+\rangle, V|-\rangle\}$ (or vice versa): Then, since

$$U_R U_X U_R^\dagger = s_1 U_Y, \quad U_R U_Y U_R^\dagger = s_2 U_Z \tag{A12}$$

(s_1 and s_2 arbitrary signs) all of the U_G for $G = X, Y, Z$ would be antidiagonal in one of the two bases, but this violates the algebra of $D_2 \equiv \{I, X, Y, Z\}$ in A_4. Accordingly, choosing the $\{|+\rangle, |-\rangle\}$ basis and imposing

$$U_X U_Y = t_1 U_Y U_X = t_2 U_Z, \quad U_G^2 = t_3 I \tag{A13}$$

(for $G = X, Y, Z$ and t_1, t_2, t_3 arbitrary signs), it is easy to see that up to a change of basis we can always take

$$U_G = i\sigma_G, \quad G = X, Y, Z,$$

with $|+\rangle$ and $|-\rangle$ eigenvectors of σ_Z. This implies that, in order to satisfy (A12), U_R cannot have vanishing elements in $\{|+\rangle, |-\rangle\}$ and then by Eq. (A11) it must be diagonal in $\{V|+\rangle, V|-\rangle\}$. Consequently, we must have

$$U_R := VDV^\dagger, \tag{A14}$$

where $D = \mathrm{diag}(e^{i\epsilon}, e^{-i\epsilon})$ in $\{|+\rangle, |-\rangle\}$ and $e^{3i\epsilon}$ is a sign. As a consequence, using conditions (A13), one sees that the U_X, U_Y, and U_Z cannot have vanishing elements in $\{V|+\rangle, V|-\rangle\}$. This in turn implies, by Eq. (A12), that V cannot have vanishing elements in $\{|+\rangle, |-\rangle\}$.

Let us now pose

$$V = \begin{pmatrix} \rho e^{i\theta} & \tau e^{i\varphi} \\ -\tau e^{-i\varphi} & \rho e^{-i\theta} \end{pmatrix} : \rho,\tau > 0, \quad \rho^2 + \tau^2 = 1.$$

Multiplying the unitarity condition on the left by $A^\dagger_{-I}$,

$$A_I A^\dagger_{RX} + A_{-RX} A^\dagger_{-I} + A_R A^\dagger_Y + A_{-Y} A^\dagger_{-R} = 0,$$

and recalling that $A^\dagger_{-I} A_R A^\dagger_Y = 0$ by Eq. (A14), one has

$$A^\dagger_{-I} A_{-RX} A^\dagger_{-I} + A^\dagger_{-I} A_{-Y} A^\dagger_{-R} = 0.$$

Now substituting Eq. (A10) and using the definition (A9), the nonvanishing matrix element of the previous identity in the basis $\{|+\rangle,|-\rangle\}$ is

$$\langle -|V^\dagger U_{RX} V|-\rangle\langle -|U^\dagger_{RX}|-\rangle = -e^{i\epsilon}\langle -|V^\dagger U_Y V|-\rangle\langle -|U^\dagger_Y U_R|-\rangle.$$

Recalling the form of V given above and using the fact that $U_{RX} = t' U_R U_X$ (t' a sign) and that U_R cannot have vanishing elements in the basis $\{|+\rangle,|-\rangle\}$, for the previous equation we finally obtain

$$\cos(\theta_1 + \varphi_1) = -i\,\sin(\theta_1 + \varphi_1) e^{2i\epsilon},$$

which has no solution.

3. Exclusion of $\mathbb{Z}_n$, D_n, $\mathbb{Z}_n \times \mathbb{Z}_2$, and $D_n \times \mathbb{Z}_2$, with $n = 3,4,6$

The aim of the present section is (1) to construct the real, orthogonal, and three-dimensional faithful representations of the groups $L \in \{\mathbb{Z}_n, D_n, \mathbb{Z}_n \times \mathbb{Z}_2, D_n \times \mathbb{Z}_2 | n = 3,4,6\}$ and (2) to exclude all the graphs arising from L by means of the unitarity conditions.

By the classification theorem for real matrices of finite order given in Ref. [28], any matrix in O(3) of order n is similar to one of the form

$$R_{\theta,s} := \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & s \end{pmatrix},$$

with $\theta = \frac{2z\pi}{n}$, z an integer, and s a sign. The matrices $R_{\theta,s}$ represent the generators for the subgroups of order $n = 3,4,6$ in L. We can generate the orbits of L starting from the generic vector (up to a rotation around the z axis) given by $\mathbf{v}_1 = (1,0,h)^T$. It is easy to show that the only matrices in O(3) of order 2 commuting with $R_{\theta,s}$ for all θ and s are $R_{0,t}$ and $R_{\pi,t}$: They represent the generators of $L/\mathbb{Z}_n$ for $L \cong \mathbb{Z}_n \times \mathbb{Z}_2$ or L/D_n for $L \cong D_n \times \mathbb{Z}_2$. On the other hand, the involutions

$$S_{\varphi,r} := \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ \sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & r \end{pmatrix}$$

are the only ones such that $S_{\varphi,r} R_{\theta,s} S^{-1}_{\varphi,r} = S_{\varphi,r} R_{\theta,s} S_{\varphi,r} = R^{-1}_{\theta,s}$. This implies that the $S_{\varphi,r}$ represent the generators for the subgroups of reflections when L is a dihedral group. Therefore, in general, the elements of $\mathcal{O}_L(\mathbf{v}_1)$ lie on the two circumferences which are parallel to the xy plane at heights $z = \pm h$.

In order to solve the unitarity conditions, it is necessary to determine the paths with length 2 constructed by elements in $\{\mathbf{0}\} \cup \mathcal{O}_L(\mathbf{v}_1)$: By the above analysis, the problem is reduced to a two-dimensional problem, since the form of the vectors in $\mathcal{O}_L(\mathbf{v}_1)$ is $\mathbf{v}_i = (x_i, y_i, \pm h)^T := (\cos\chi_i, \sin\chi_i, \pm h)^T$. Accordingly, it is easy to see that

$$\mathbf{v}_i \pm \mathbf{v}_j = s\mathbf{v}_l + t\mathbf{v}_p, \quad \mathbf{v}_i,\mathbf{v}_j,\mathbf{v}_l,\mathbf{v}_p \neq \mathbf{0} \quad (s,t \text{ signs})$$

implies $(x_i, y_i) = s(x_l, y_l)$ or $(x_i, y_i) = t(x_p, y_p)$.

(a) Case $n = 4$. There are at least two inequivalent orthogonal representations of $L \in \{\mathbb{Z}_4, D_4, \mathbb{Z}_4 \times \mathbb{Z}_2, D_4 \times \mathbb{Z}_2\}$, since the element of order 4 can be represented by either $R_{\pi/2,-}$ or $R_{\pi/2,+}$. We will now analyze the two different cases.

In the first $R_{\pi/2,-}$ generates the four vectors

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \\ h \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 0 \\ 1 \\ -h \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} -1 \\ 0 \\ h \end{pmatrix}, \quad \mathbf{v}_4 = \begin{pmatrix} 0 \\ -1 \\ -h \end{pmatrix}.$$

The differences $\mathbf{v}_i - \mathbf{v}_j \neq 0\ \forall i,j \in \{1,2,3,4\}$ are uniquely determined as sums of elements of $\{\mathbf{0}, \mathcal{O}_L(\pm\mathbf{v}_1)\}$. Accordingly, there is a cyclic subgroup of order 4 (i.e., $\mathbb{Z}_4$) whose orbit satisfies Eq. (14) and thus, invoking Proposition 3 (we recall that the representation U must be faithful), we exclude the representation containing $R_{\pi/2,-}$.

Taking now $R_{\pi/2,+}$, the orbit is

$$\mathbf{v}_1 = \begin{pmatrix} 1 \\ 0 \\ h \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} 0 \\ 1 \\ h \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} -1 \\ 0 \\ h \end{pmatrix}, \quad \mathbf{v}_4 = \begin{pmatrix} 0 \\ -1 \\ h \end{pmatrix}.$$

We have that the vectors

$$\mathbf{v}_1 + \mathbf{v}_2, \quad \mathbf{v}_1 - \mathbf{v}_3 \tag{A15}$$

are uniquely determined as sum of elements of $\{\mathbf{0}, \mathcal{O}_L(\pm\mathbf{v}_1)\}$. Let us denote by R the matrix representing $R_{\pi/2,+}$ in SU(2) and proceed as in Sec. 2. From now on in the present section we use the notation of Eq. (A9) and perform calculations in the $\{|+\rangle,|-\rangle\}$ basis. Multiplying the unitarity conditions associated with the vectors in (A15) on the right by $A_{\mathbf{v}_1}$, we obtain

$$A_{\mathbf{v}_1} R A^\dagger_{-\mathbf{v}_1} R^\dagger A_{\mathbf{v}_1} = 0, \quad A_{\mathbf{v}_1} R^2 A^\dagger_{\mathbf{v}_1} R^{2\dagger} A_{\mathbf{v}_1} = 0. \tag{A16}$$

By the first of conditions (A16), up to a change of basis we can impose

$$R = \begin{pmatrix} \mu & 0 \\ 0 & \mu^* \end{pmatrix}, \quad R^4 = sI$$

(s arbitrary sign); using the second condition, it follows that

$$R^2 = \begin{pmatrix} \mu^2 & 0 \\ 0 & \mu^{*2} \end{pmatrix} = V \begin{pmatrix} 0 & \nu \\ -\nu^* & 0 \end{pmatrix} V^\dagger \tag{A17}$$

and thus necessarily $\mu^2 \neq \mu^{*2}$. Consider now the unitarity condition

$$A_{\mathbf{v}_1} A^\dagger_{\mathbf{v}_2} + A_{-\mathbf{v}_2} A^\dagger_{-\mathbf{v}_1} + A_{\mathbf{v}_4} A^\dagger_{\mathbf{v}_3} + A_{-\mathbf{v}_3} A^\dagger_{-\mathbf{v}_4} = 0.$$

Multiplying this last equation by $A_{\mathbf{v}_1}$ on the right and taking the adjoint we get[4]

$$A^\dagger_{\mathbf{v}_1}A_{\mathbf{v}_2}A^\dagger_{\mathbf{v}_1} + A^\dagger_{\mathbf{v}_1}A_{-\mathbf{v}_4}A^\dagger_{-\mathbf{v}_3} = 0,$$

which amounts to

$$\frac{\alpha_+^2}{\alpha_-^2}\langle +|R^\dagger|+\rangle\langle +|V^\dagger RV|+\rangle = -\nu^*\langle -|R^\dagger|-\rangle\langle +|V^\dagger R^3 V|-\rangle. \quad \text{(A18)}$$

Posing now

$$V^\dagger RV = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

with $a,b \neq 0$ since otherwise $V^\dagger R^2 V$ cannot be antidiagonal [see (A17)], we have that

$$V^\dagger R^3 V = (V^\dagger RV)(V^\dagger R^2 V) = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix}\begin{pmatrix} 0 & \nu \\ -\nu^* & 0 \end{pmatrix}.$$

Accordingly, Eq. (A18) leads to

$$\frac{\alpha_+^2}{\alpha_-^2} = -\mu^2,$$

which is impossible, since $\mu^2 \neq \mu^{*2}$.

(b) Cases $n = 3,6$. The representations of $L \in \{\mathbb{Z}_n, D_n, \mathbb{Z}_n \times \mathbb{Z}_2, D_n \times \mathbb{Z}_2 | n = 3,6\}$ must contain $R_{2\pi/3,+}$, which generates a subgroup K isomorphic to $\mathbb{Z}_3$: $\mathcal{O}_K(\mathbf{v}_1)$ is given by the following vectors:

$$\mathbf{v}_l = \begin{pmatrix} \cos\frac{2\pi}{3}(l-1) \\ \sin\frac{2\pi}{3}(l-1) \\ h \end{pmatrix}, \quad l \in \{1,2,3\}.$$

We denote the representation matrix of $R_{2\pi/3,+}$ in SU(2) by $U_{2\pi/3}$.

If $\mathbf{v}_1 - \mathbf{v}_2$ is uniquely determined as the sum of elements of $\{\mathbf{0}, \mathcal{O}_L(\pm\mathbf{v}_1)\}$ (a particular case is given by the condition $h = 0$), we can exclude this case by Proposition 6. Let us then suppose that $\mathbf{v}_1 - \mathbf{v}_2$ is not uniquely determined as the sum of elements of $\{\mathbf{0}, \mathcal{O}_L(\pm\mathbf{v}_1)\}$ (in particular $h \neq 0$). Then, by the above analysis, $\mathcal{O}_L(\mathbf{v}_1)$ must contain

$$\mathbf{v}_l = \begin{pmatrix} -\cos\frac{2\pi}{3}(l-1) \\ -\sin\frac{2\pi}{3}(l-1) \\ h \end{pmatrix}, \quad l \in \{4,5,6\}$$

(such that $\mathbf{v}_1 - \mathbf{v}_2 = \mathbf{v}_5 - \mathbf{v}_4$). Again, via the above arguments on the representations of L, it is easy to see that $\mathbf{v}_1 + \mathbf{v}_2$ is uniquely determined as the sum of elements of $\{\mathbf{0}, \mathcal{O}_L(\pm\mathbf{v}_1)\}$. Then, from the condition

$$A_{\mathbf{v}_1}A^\dagger_{-\mathbf{v}_2} + A_{\mathbf{v}_2}A^\dagger_{-\mathbf{v}_1} = 0,$$

by multiplying on the right by $A_{\mathbf{v}_1}$, we get

$$A_{\mathbf{v}_1}A^\dagger_{-\mathbf{v}_2}A_{\mathbf{v}_1} = 0.$$

[4]One has $A_{-\mathbf{v}_2}A^\dagger_{-\mathbf{v}_1}A_{\mathbf{v}_1} = 0$, since $A^\dagger_{-\mathbf{v}_1}A_{\mathbf{v}_1} = 0$, and $A_{\mathbf{v}_4}A^\dagger_{\mathbf{v}_3}A_{\mathbf{v}_1} = 0$, since $A^\dagger_{\mathbf{v}_3}A_{\mathbf{v}_1} = R^2 A^\dagger_{\mathbf{v}_1}R^{2\dagger}A_{\mathbf{v}_1}$ and $A^\dagger_{\mathbf{v}_1}R^2 A_{\mathbf{v}_1} = \alpha_+^2|+\rangle\langle +|V^\dagger R^2 V|+\rangle\langle +|$, and by Eq. (A17), $\langle +|V^\dagger R^2 V|+\rangle = 0$.

Up to a change of basis $U_{2\pi/3} = \mathrm{diag}(e^{i\epsilon}, e^{-i\epsilon})$ holds with $e^{3i\epsilon} = \pm 1$ and $\epsilon \notin \{0,\pi\}$. Let U_π represent the element of L mapping $\mathbf{v}_1$ to $\mathbf{v}_4$. This element is an involution and there are only two cases (by inspection of the groups L here considered)

$$U_\pi U_{2\pi/3}U^\dagger_\pi = sU_{2\pi/3} = s'U^\dagger_{2\pi/3} \quad \text{(A19)}$$

(s,s' signs). Recalling that the representation $U \subset \mathrm{SU}(2)$ is faithful and $U^3_{2\pi/3} = tI$ (t a sign), it is easy to verify that the previous two conditions on $U_{2\pi/3}$ and U_π are satisfied, respectively, only if (1) U_π is diagonal and (2) U_π is antidiagonal. Multiplying the unitarity condition associated with the difference $\mathbf{v}_1 - \mathbf{v}_4$ by $A_{\mathbf{v}_1}$ on the right,

$$A_{\mathbf{v}_1}A^\dagger_{\mathbf{v}_4} + A_{-\mathbf{v}_4}A^\dagger_{-\mathbf{v}_1} = 0,$$

one also gets

$$A_{\mathbf{v}_1}A^\dagger_{\mathbf{v}_4}A_{\mathbf{v}_1} = 0,$$

namely, either $A^\dagger_{\mathbf{v}_4}A_{\mathbf{v}_1} = 0$ or $A_{\mathbf{v}_1}A^\dagger_{\mathbf{v}_4} = 0$. This implies that (a) $V^\dagger U_\pi V$ is antidiagonal or (b) U_π is antidiagonal. In case (a), multiplying the unitarity condition by $A_{\mathbf{v}_1}$ on the right,

$$A_{\mathbf{v}_1}A^\dagger_{\mathbf{v}_2} + A_{-\mathbf{v}_2}A^\dagger_{-\mathbf{v}_1} + A_{\mathbf{v}_5}A^\dagger_{\mathbf{v}_4} + A_{-\mathbf{v}_4}A^\dagger_{-\mathbf{v}_5} = 0,$$

it follows that

$$A_{\mathbf{v}_1}A^\dagger_{\mathbf{v}_2}A_{\mathbf{v}_1} + A_{-\mathbf{v}_4}A^\dagger_{-\mathbf{v}_5}A_{\mathbf{v}_1} = 0; \quad \text{(A20)}$$

in case (b) multiplying the unitarity condition by $A^\dagger_{\mathbf{v}_1}$ on the right,

$$A^\dagger_{\mathbf{v}_1}A_{\mathbf{v}_2} + A^\dagger_{-\mathbf{v}_2}A_{-\mathbf{v}_1} + A^\dagger_{\mathbf{v}_5}A_{\mathbf{v}_4} + A^\dagger_{-\mathbf{v}_4}A_{-\mathbf{v}_5} = 0, \quad \text{(A21)}$$

and taking the adjoint, it follows that

$$A_{\mathbf{v}_1}A^\dagger_{\mathbf{v}_2}A_{\mathbf{v}_1} + A_{\mathbf{1}}A^\dagger_{-\mathbf{v}_5}A_{-\mathbf{v}_4} = 0. \quad \text{(A22)}$$

Let us now pose

$$V^\dagger U_{2\pi/3}V = \begin{pmatrix} a & b \\ -b^* & a^* \end{pmatrix},$$

where $a \neq 0$ since $U^3_{2\pi/3} = tI$. In case (a), from (A20) one then has

$$\frac{\alpha_+^2}{\alpha_-^2}e^{i\epsilon} = -\langle -|U^\dagger_\pi U_{2\pi/3}U_\pi|-\rangle,$$

which cannot be satisfied in either case 1 or case 2. On the other hand, in case (b), from (A22) one has

$$\frac{\alpha_+^2}{\alpha_-^2}a^* e^{i\epsilon} = -e^{-i\epsilon}\langle -|V^\dagger U^\dagger_\pi U^\dagger_{2\pi/3}U_\pi V|-\rangle,$$

and since U_π is antidiagonal, one has

$$\frac{\alpha_+^2}{\alpha_-^2}a^* e^{2i\epsilon} = -\langle -|V^\dagger U_{2\pi/3}V|-\rangle = -a^*,$$

which is impossible, since $e^{3i\epsilon} = \pm 1$ for $\epsilon \notin \{0,\pi\}$.

4. Remaining presentations arising from $\mathbb{Z}_2$, D_2, and $D_2 \times \mathbb{Z}_2$

By the argument of Sec. 3, any matrix of order 2 in O(3) is similar to

$$M_{s,t} := \begin{pmatrix} s & 0 & 0 \\ 0 & s & 0 \\ 0 & 0 & t \end{pmatrix},$$

with s,t signs. Accordingly, up to conjugation, any three-dimensional orthogonal representation of a group $L \in \{\mathbb{Z}_2, D_2, D_2 \times \mathbb{Z}_2\}$ contains $M_{s,t}$. If $s \neq t$, any matrix N of order 2 in O(3) commuting with $M_{s,t}$ is either $M_{s',t'}$ or of the form

$$N = \begin{pmatrix} \cos\varphi & \sin\varphi & 0 \\ \sin\varphi & -\cos\varphi & 0 \\ 0 & 0 & r \end{pmatrix},$$

with r a sign. Since the two-dimensional block is a reflection matrix, there exists a similarity transformation which maps it to $\pm\sigma_z$ (and leaving $M_{s,t}$ invariant). Thus the real, orthogonal, and three-dimensional faithful representations of the groups here considered contain just $M_{s,t}$ and

$$N_{r_1,r_2} := \begin{pmatrix} r_1 & 0 & 0 \\ 0 & -r_1 & 0 \\ 0 & 0 & r_2 \end{pmatrix}.$$

The problem reduces to combine signs in $M_{s,t}$ and N_{r_1,r_2} to give rise to faithful representations of L. It is easy to check that they give rise to the integer lattice, the square lattice, or the bcc lattice (one can include the inverses or not). Nevertheless, there are two ways of providing a minimal generating set (namely, such that $S_+ \neq S_-$) for $\mathbb{Z}^3$ and whose Cayley graph is associated with the bcc lattice. Such presentations are both generated by D_2: One is made with the vertices of a tetrahedron; the second one corresponds to the vertices given by the vectors

$$\mathbf{v}_0 = \begin{pmatrix} 1 \\ 1 \\ h \end{pmatrix}, \quad \mathbf{v}_1 = \begin{pmatrix} -1 \\ -1 \\ h \end{pmatrix}, \quad \mathbf{v}_2 = \begin{pmatrix} -1 \\ 1 \\ h \end{pmatrix}, \quad \mathbf{v}_3 = \begin{pmatrix} 1 \\ -1 \\ h \end{pmatrix}.$$

We notice that excluding this solution allows us to exclude the case including the inverses, namely, $S_+ = S_-$.

From the unitarity conditions one has

$$A_{\mathbf{v}_0} A^\dagger_{\mathbf{v}_1} A_{\mathbf{v}_0} = 0, \tag{A23}$$

$$A_{\mathbf{v}_0} A^\dagger_{-\mathbf{v}_i} A_{\mathbf{v}_0} = 0, \quad i = 2,3 \tag{A24}$$

$$A_{\mathbf{v}_0} A^\dagger_{-\mathbf{v}_1} + A_{\mathbf{v}_1} A^\dagger_{-\mathbf{v}_0} + A_{\mathbf{v}_2} A^\dagger_{-\mathbf{v}_3} + A_{\mathbf{v}_3} A^\dagger_{-\mathbf{v}_2} = 0. \tag{A25}$$

From (A23) and the form of Eqs. (A9) and (A10) for the transition matrices, we get $U_1 = i\sigma_1$ (we use the equivalent notation for Pauli matrices $\sigma_0 := I$, $\sigma_1 := \sigma_X$, $\sigma_2 := \sigma_Y$, and $\sigma_3 := \sigma_Z$), up to a change of basis; from (A24) we end up with the two cases (1) $A^\dagger_{-\mathbf{v}_2} A_{\mathbf{v}_0} = A^\dagger_{-\mathbf{v}_3} A_{\mathbf{v}_0} = 0$ and (2) $A^\dagger_{-\mathbf{v}_2} A_{\mathbf{v}_0} = A_{\mathbf{v}_0} A^\dagger_{-\mathbf{v}_3} = 0$, since $A_{\mathbf{v}_0} A^\dagger_{-\mathbf{v}_2} = A_{\mathbf{v}_0} A^\dagger_{-\mathbf{v}_3} = 0$ is forbidden in order to respect the D_2 algebra, while the case $A^\dagger_{-\mathbf{v}_3} A_{\mathbf{v}_0} = A_{\mathbf{v}_0} A^\dagger_{-\mathbf{v}_2} = 0$ is accounted for by the symmetry of the unitarity conditions under the exchange $2 \leftrightarrow 3$. In case 1, the condition is incompatible with a faithful representation of D_2 in SU(2). In case 2, we have $U_G = i\sigma_G$ and $U_2 = VDV^\dagger$ with D diagonal, implying that $U_2 = sV(i\sigma_3)V^\dagger$ (s a sign). Then, up to a global sign, one has

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} i & s \\ -s & -i \end{pmatrix},$$

and from (A25) we obtain

$$A_{\mathbf{v}_0} A^\dagger_{-\mathbf{v}_1} A_{\mathbf{v}_0} + A_{\mathbf{v}_2} A^\dagger_{-\mathbf{v}_3} A_{\mathbf{v}_0} = 0,$$

which, using the form of Eqs. (A9) and (A10) for the transition matrices along with the previous results, leads to $-2\alpha_+^2\alpha_- = 0$, contradicting the assumption $\alpha_\pm \neq 0$.

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