Massless interacting fermionic cellular automaton exhibiting bound states

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We present a fermionic cellular automaton model which describes massless Dirac fermions in $1+1$ dimension coupled with local, number preserving interaction. The diagonalization of the two particle sector shows that specific values of the total momentum and of the coupling constant allow for the formation of bound states. Furthermore, we present a classification of the local number preserving interactions that are invariant under the isotropy group of the cellular automaton which simulates the Weyl equation.

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I. INTRODUCTION

Quantum cellular automata (QCAs) [1–4] are the most general unitary dynamics of a lattice of quantum systems which is discrete in time and local, namely, the speed of information propagation is bounded. The idea of QCAs can be traced back to the seminal work of Feynman [5] where QCAs were introduced as quantum simulators. Since then, QCAs have been considered as a paradigm for quantum computation [6–9] and have been applied to the study of many-body quantum systems [10–15].

Nevertheless, quantum simulation still is a major application of QCAs, in particular as discretized quantum field theories. Many authors [16–24] studied the simulation of noninteracting quantum field theories with discrete-time quantum walks (QWs) [25,26], which are the single-particle restriction of bosonic QCAs or fermionic cellular automata (FCAs)—a variation of QCAs where the cells correspond to arrays of local fermionic modes [27]. Indeed, a QW describes the most general discrete-time evolution of a single particle on a lattice which is unitary and local, i.e., at each step the particle can move at most by a bounded number of lattice sites. More recently, the focus shifted towards models in which the particles interact with an external potential [28–31] and towards interacting field theories [32,33].

Intuitively, we expect that a QCA or FCA which simulates (or recovers) a given continuous dynamics is such that, if we restrict to sufficiently smeared states which cannot probe the discreteness of the lattice, we cannot tell the evolution apart from the dynamics of a field on a continuous space. For the noninteracting case this behavior is rather well understood. In the limit of small masses and momentum, where we can neglect powers of m and k beyond the linear terms, and interpolating discrete time steps with a continuous time direction, the evolution of the cellular automaton is described by a relativistic wave equation. The interacting case, still rather unexplored, is significantly different. The intrinsic discreteness of cellular automata may produce phenomenological features with no counterpart in the continuum and that do not vanish in the large scale limit, like a different set of bound states and scattering processes that conserve energy only up to integer multiples of an additive constant (indeed, if time is discrete, energy is defined only modulo to the addition of integer multiples of 2π, and can thus be reduced in the interval $[-\pi, \pi]$) [32,34].

In this paper we classify the family of local and number preserving interactions which are invariant under the isotropy group of the Weyl automaton, namely, the fermionic cellular automaton which recovers the Weyl equation in $3+1$ dimensions.

Then we study an interacting $(1+1)$-dimensional FCA given by the composition of a free evolution, which is modeled after the massless Dirac equation [20] followed by a quartic, number preserving local interaction. We chose this interaction among the isotropic ones that we classified.

We will study the evolution of the two-particle sector by providing the spectral resolution of the unitary evolution corresponding to a single step of the FCA. Our analysis will show that, even if the free theory is gapless and the interaction is a compact perturbation, bound states appear for critical values of the total momentum and of the coupling constant.

In Sec. II we review the technical tools employed for QCAs and QWs and provide a mathematical description of the Dirac automaton.

In Sec. III we provide the classification of all the suitable local, isotropic, and number preserving interactions for our automaton, in particular for the two-particle sector, and we describe the interaction considered among the ones derived and its properties; then we derive the scattering and the bounded

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states of the system. In Appendixes A and B we check the completeness of the solution set.

II. FERMIONIC CELLULAR AUTOMATA

A QCA [3] describes the single step unitary evolution $\mathcal{U}$ of a set Γ of cells each of which represents a quantum system. Usually, every cell consists in a d-level system. However, we are interested in FCAs, where every cell corresponds to s local fermionic modes [35,36], represented by the field operators $\psi_{x,a}$, $a = 1, \dots, s$ obeying the canonical anticommutation relations:

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

The N-particle states can be described by introducing the Fock space representation $|(x_1, a_1), \dots, (x_N, a_N)\rangle := \psi^\dagger_{x_1,a_1} \dots \psi^\dagger_{x_N,a_N}|\Omega\rangle$, where $|\Omega\rangle$ is the *vacuum state*. The state $|\Omega\rangle$ is defined by the identity $\psi_{x,a}|\Omega\rangle = 0$ for all i and it is the state with no particles. Here, we chose the representation in which the vacuum state is the one with no *localized* excitations, whereas in quantum field theory the vacuum state is usually the ground state of a free Hamiltonian.

Linear FCA with symmetries: Weyl and Dirac automata

In the particular case of a free, i.e., noninteracting, evolution, the FCA is linear in the field operators, namely, $\mathcal{U}(\psi^\dagger_{x,a}) = \sum_{y,b} U^{y,b}_{x,a}\psi_{y,b}$ for some complex coefficients $U^{y,b}_{x,a}$ and the number of excitations (i.e., particles) is conserved. Therefore, the dynamics is completely specified by a *quantum walk* on the one-particle sector:

$$\begin{aligned} &|\phi(t+1)\rangle = \mathbf{U}|\phi(t)\rangle, \\ &\mathbf{U} \in \mathcal{L}(\mathcal{H}_1), \ \mathcal{H}_1 := \mathrm{span}\{|x, a\rangle\} \equiv \ell^2(\Gamma) \otimes \mathbb{C}^s, \\ &\mathbf{U} := \sum_{x,y,a,b} U^{y,b}_{x,a}\, |x\rangle\langle y| \otimes |a\rangle\langle b|, \end{aligned} \tag{2}$$

where we use the isomorphism $|x, a\rangle \leftrightarrow |a\rangle|x\rangle$. Accordingly, the n-particle sector of a linear FCA $\mathcal{U}$ is described by the total antisymmetric subspace of the n-particle quantum walk $\mathbf{U}^{\otimes n}$. Therefore, a linear FCA can be regarded as the second quantization of a quantum walk.

The FCA evolution must also be *local*, namely, for a fixed $x \in \Gamma$ $U^{y,b}_{x,a} \neq 0$ only for finitely many $y \in \Gamma$, which are called the *neighbors* of x (see Fig. 1). From this locality assumption, we have that the set G is naturally endowed with a graph structure, where $x \in \Gamma$ are the vertices and there is an edge between a cell and its neighbors.

In the most general case, the update rule may change from cell to cell [4]. However, it is reasonable to assume a *homogeneous* evolution, with the same update rule for every cell. More precisely, the homogeneity assumption requires [20,37] that the graph Γ is the Cayley graph of a group G that can be presented as $G = \langle S|R\rangle$ where S is a finite set of generators and R is a finite set of relators. Each edge connecting a cell x with its neighbors corresponds to an element of S and elements of R correspond to closed paths on the graph. If a linear FCA is local and homogeneous the unitary operator $\mathbf{U}$

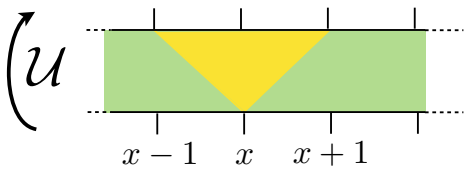

FIG. 1. In a one-dimensional cellular automaton each cell is labeled by an integer number x and the one-step time evolution is described by a unitary operator $\mathcal{U}$. In a nearest-neighbor one-dimensional QCA the state of the cell x at time $t+1$ depends only on the state of the cells $x-1$, x, and $x+1$ at time t. Because of the locality of the evolution, information cannot propagate at an arbitrary speed: physical interventions on cell x can only affect the state of the cells lying in the future light cone of x (in yellow).

of Eq. (24) can be written as follows:

$$\mathbf{U} := \sum_{h\in S} \mathbf{T}_h \otimes \mathbf{U}_h \tag{3}$$

where $\mathbf{T}$ is the right regular representation of G on $\ell^2(G)$ acting as $\mathbf{T}_h|x\rangle := |xh^{-1}\rangle$ and $\mathbf{U}_h \in \mathcal{L}(\mathbb{C}^s)$.

Let us now review a notion of *isotropy* [38] for a FCA as in Eq. (3). Let us consider a decomposition $S = S_+ \cup s_- \cup \{e\}$ of the set of generators (e denotes the identity on G), let L be a group of graph automorphisms that is transitive over S_+, and let $\mathbf{V} : L \to \mathcal{L}(\mathbb{C}^s)$ be a faithful projective representation of L. Then, we say that $\mathbf{U}$ is isotropic if the following covariance condition holds:

$$\mathbf{U} = \sum_{h\in S} \mathbf{T}_h \otimes \mathbf{U}_h = \sum_{h\in S} \mathbf{T}_h \otimes \mathbf{V}_l\mathbf{U}_h\mathbf{V}_l^\dagger, \quad \forall l \in L. \tag{4}$$

Generally, the same FCA on the Cayley graph corresponding to the presentation $G = \langle S|R\rangle$ might satisfy isotropy for one or more choices of the set S_+, group L, and representation $\mathbf{U}$. For a given S, different choices of S_+ correspond to different orientations of some edges over the same graph.

The Cayley graph Γ can be endowed with the word metric: the distance between x and y is equal to the length of the shortest path connecting x and y. If the dynamics of a free fermionic field on flat spacetime is expected to emerge as a large scale description of the FCA, then Γ must be quasi-isometrically embeddable [39] in the Euclidean space $\mathbb{R}^3$. A well-known result in geometric group theory [40] states that a group G is quasi-isometrically embeddable in $\mathbb{R}^n$ space if and only if it has a subgroup isomorphic to $\mathbb{Z}^n$ of finite index.

Let us now restrict ourselves to the case $G = \mathbb{Z}^3$ and to FCAs with two fermionic degrees of freedom per cell ($s = 2$). Then, the only graph which admits an isotropic linear FCA is the bcc lattice [38] and we only have the following two isotropic linear FCAs (see Fig. 2):

$$\mathbf{W}^{(\pm)} := \sum_{h\in S} \mathbf{T}_h \otimes \mathbf{W}^{(\pm)}_h, \tag{5}$$

$$\begin{aligned} &\mathbf{W}^{(\pm)}_{h_1} := \begin{pmatrix} \eta^\pm & 0 \\ \eta^\pm & 0 \end{pmatrix}, \quad \mathbf{W}^{(\pm)}_{-h_1} := \begin{pmatrix} 0 & -\eta^\mp \\ 0 & \eta^\mp \end{pmatrix}, \\ &\mathbf{W}^{(\pm)}_{\pm h_2} := \sigma_x\mathbf{W}^{(\pm)}_{\pm h_1}\sigma_x, \quad \mathbf{W}^{(\pm)}_{\pm h_3} := \sigma_y\mathbf{W}^{(\pm)}_{h_1}\sigma_y, \\ &\mathbf{W}^{(\pm)}_{\pm h_4} := \sigma_z\mathbf{W}^{(\pm)}_{h_1}\sigma_z, \quad \eta^\pm := \frac{1 \pm i}{4}, \end{aligned} \tag{6}$$

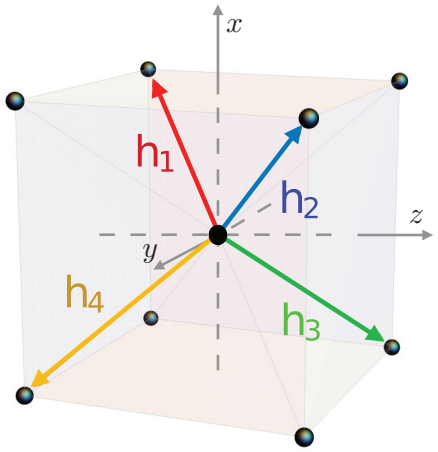

FIG. 2. The bcc lattice is the Cayley graph of $\mathbb{Z}^3$ corresponding to the presentation $\mathbb{Z}^3 = \langle h_1, h_2, h_3, h_4 | h_1 + h_2 + h_3 + h_4 \rangle$ (the Abelian relators are omitted). The isotropy group is the π rotation around the x, y, and z axis, i.e., $L := \{I, R(\pi, x), R(\pi, y), R(\pi, z)\}$.

with $S_+ = \{h_1, h_2, h_3, h_4\}$ and the nontrivial relator $h_1 + h_2 + h_3 + h_4 = 0$. Given an orthonormal reference frame, the generators can be chosen as follows (see Fig. 2):

$$h_1 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\-1\\-1\end{pmatrix}, \quad h_2 = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix},$$
$$h_3 = \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\-1\\1\end{pmatrix}, \quad h_4 = \frac{1}{\sqrt{3}}\begin{pmatrix}-1\\1\\-1\end{pmatrix}. \tag{7}$$

The isotropy group of W is the subgroup of SO(3) given by the the π rotation around the x, y, and z axis, and we have the usual spin-1/2 representation on the internal degrees of freedom, i.e.,

$$L := \{I, R(\pi, x), R(\pi, y), R(\pi, z), \}, \tag{8}$$

$$\mathbf{V}^W_I = I, \quad \mathbf{V}^W_{R(\pi,x)} = i\sigma_x,$$
$$\mathbf{V}^W_{R(\pi,y)} = i\sigma_y, \quad \mathbf{V}^W_{R(\pi,z)} = i\sigma_z. \tag{9}$$

For the Abelian group $\mathbb{Z}^3$, the homogeneity assumption is the usual translation invariance. It is therefore convenient to introduce the the Fourier transform of the local modes:

$$\psi^\dagger_{k,a} := \sum_x e^{-ik\cdot x}\psi^\dagger_{x,a}, \quad k \in B, \tag{10}$$

where B denotes the Brillouin zone of the bcc lattice. Then, a generic one-particle state can be written as $|\phi\rangle = \int_B dk \sum_a \tilde{c}_{a,k}|a\rangle|k\rangle$ with $|k\rangle := \sum_x e^{-ik\cdot x}|x\rangle$ and the unitary operator of Eq. (5) becomes [20]

$$\mathbf{W}^{(\pm)} = \int_B dk|k\rangle\langle k| \otimes \mathbf{W}^{(\pm)}(k), \tag{11}$$
$$\mathbf{W}^{(\pm)}(k) = d^{(\pm)}(k)I - ia^{(\pm)}_x(k)\sigma_x + \pm ia^{(\pm)}_y(k)\sigma_y + -ia^{(\pm)}_z(k)\sigma_z, \tag{12}$$

$$d^{(\pm)}(k) := c_x c_y c_z \mp s_x s_y s_z,$$
$$a^{(\pm)}_x(k) := s_x c_y c_z \pm c_x s_y s_z,$$
$$a^{(\pm)}_y(k) := c_x s_y c_z \mp s_x c_y s_z,$$
$$a^{(\pm)}_z(k) := c_x c_y s_z \pm s_x s_y c_z, \tag{13}$$

$$c_i := \cos\tfrac{k_i}{\sqrt{3}}, \quad s_i := \cos\tfrac{k_i}{\sqrt{3}}. \tag{14}$$

One could verify [20] that, in the limit $k \to 0$, we have $\mathbf{W}^{(\pm)}(k) \approx \exp[-iH^\pm_W(k)]$ where $H^+_W(k)$ is the Hamiltonian of the right-handed Weyl equation and $H^-_W(k)$ is the Hamiltonian of the left-handed Weyl equation (up to a change of coordinates). Therefore, the FCA in Eq. (5) is called the Weyl cellular automaton. The Dirac automaton arises [20] from the local coupling of two Weyl automata in a direct sum:

$$\mathbf{D} := \int_B dk|k\rangle\langle k| \otimes \mathbf{D}(k), \tag{15}$$
$$\mathbf{D}(k) := \begin{pmatrix} n\mathbf{W}(k) & imI \\ imI & n\mathbf{W}^\dagger(k)\end{pmatrix},$$
$$n^2 + m^2 = 1, \tag{16}$$

where we omitted the $\pm$ superscript in order to lighten the notation. It is easy to verify that, in the $k \to 0$ and $m \to 0$ limit, the Dirac automaton of Eq. (15) recovers the Dirac equation, with the parameter m playing the role of the rest mass.

The Dirac automaton inherits the same isotropy group L as the Weyl automata [see Eq. (8)] with the corresponding direct sum representation on the internal degrees of freedom:

$$\mathbf{V}^D_I = I, \quad \mathbf{V}^D_{R(\pi,x)} = -\sigma_x \oplus \sigma_x,$$
$$\mathbf{V}^D_{R(\pi,y)} = -\sigma_y \oplus \sigma_y, \quad \mathbf{V}^D_{R(\pi,z)} = -\sigma_z \oplus \sigma_y. \tag{17}$$

III. DIRAC AUTOMATON WITH ISOTROPIC LOCAL INTERACTIONS

In the previous section we focused on linear FCAs and QCAs. Describing an interaction, instead, involves nonlinear evolutions of the field operators. One could interpret a local interaction term as a local change of basis which models the arbitrariness of the identification of local bases at subsequent *discrete* time steps, as in a discrete version of a gauge theory. At each site x of the graph we have the action of a local gate $\exp(-iJ_x)$ where J_x is some Hermitian operator localized at site x. Then, the interaction step can be written as follows:

$$\mathcal{J}(\psi_{x,a}) := \exp(-iJ)\psi_{x,a}\exp(iJ), \quad J := \sum_x J_x. \tag{18}$$

It is natural to require that the interaction term has the same symmetries as the free evolution. For a localized interaction, translation invariance trivially implies that the interacting gate is the same at all sites. The isotropy assumption requires that the local interaction must commute with the representation of the isotropy group on the internal degrees of freedom. For the Dirac automaton of Eq. (15), the isotropy assumption implies that the interaction term commutes with the discrete rotations of Eq. (17).

In this paper, we focus our analysis on the simplest case of number preserving interactions. The most general local, isotropic, and number preserving interaction can be written as follows:

$$J_x := J_x^q + J_x^e + J_x^o, \tag{19}$$

$$\begin{aligned} J_x^q :=\ & \lambda_1(n_{x,3}\psi_{x,4}^\dagger\psi_{x,2} + n_{x,4}\psi_{x,3}^\dagger\psi_{x,1}) + \text{H.c.} \\ & + \lambda_2(n_{x,1}\psi_{x,2}^\dagger\psi_{x,4} + n_{x,2}\psi_{x,1}^\dagger\psi_{x,3}) + \text{H.c.} \\ & + \lambda_3(\psi_{x,1}^\dagger\psi_{x,2}^\dagger\psi_{x,3}\psi_{x,4}) + \text{H.c.} \\ & + \lambda_4(\psi_{x,2}^\dagger\psi_{x,4}^\dagger\psi_{x,1}\psi_{x,3} + \text{H.c.}) \\ & + \lambda_5(\psi_{x,2}^\dagger\psi_{x,3}^\dagger\psi_{x,1}\psi_{x,4} + \text{H.c.}) \\ & + \lambda_6(n_{x,1}n_{x,3} + n_{x,2}n_{x,4}) \\ & + \lambda_7(n_{x,1}n_{x,4} + n_{x,2}n_{x,3}) \\ & + \lambda_8 n_{x,1}n_{x,2} + \lambda_9 n_{x,3}n_{x,4}, \end{aligned} \tag{20}$$

$$\begin{aligned} J_x^e :=\ & \xi_1(n_{x,1}n_{x,3}\psi_{x,4}^\dagger\psi_{x,2} + n_{x,2}n_{x,4}\psi_{x,3}^\dagger\psi_{x,1}) + \text{H.c.} \\ & + \xi_2(n_{x,1} + n_{x,2})n_{x,3}n_{x,4} + \xi_3 n_{x,1}n_{x,2}(n_{x,3} + n_{x,4}), \end{aligned} \tag{21}$$

$$J_x^o := \chi n_{x,1}n_{x,2}n_{x,3}n_{x,4}, \tag{22}$$

where we introduced the number operators $n_{x,i} := \psi_{x,i}^\dagger\psi_{x,i}$. The proof of the classification has been performed through the symbolic calculation PYTHON module SYMPY and the code used is available on GitHub.

We now proceed with the phenomenological analysis of an interacting FCA. We will restrict to the easiest nontrivial case, namely, two massless four-spinors in one dimension. We thus consider a FCA model $\mathcal{A}$ of the form

$$\mathcal{A} := \mathcal{J} \circ \mathcal{F}, \tag{23}$$

where $\mathcal{F}$ is the Dirac FCA in the one-dimensional case for $m = 0$, i.e.,

$$\mathbf{F} := \int_\pi^\pi dk |k\rangle\langle k| \otimes \mathbf{F}(k), \tag{24}$$

$$\mathbf{F}(k) := \begin{pmatrix} e^{-ik} & 0 & 0 & 0 \\ 0 & e^{ik} & 0 & 0 \\ 0 & 0 & e^{ik} & 0 \\ 0 & 0 & 0 & e^{-ik} \end{pmatrix}, \tag{25}$$

or, in the position representation,

$$\begin{aligned} \mathbf{F} &= \mathbf{T} \otimes (|1\rangle\langle 1| + |4\rangle\langle 4|) + \mathbf{T}^\dagger \otimes (|2\rangle\langle 2| + |3\rangle\langle 3|), \\ \mathbf{T}|x\rangle &:= |x+1\rangle, \end{aligned} \tag{26}$$

and $\mathcal{J}$ is the interacting step (see Fig. 3). Since we are dealing with a fermionic system, the two-particle Hilbert space is given by the antisymmetric subspace $\mathcal{H}_-$ of the tensor product $\mathcal{H}_1 \otimes \mathcal{H}_1$ of two copies of the one-particle space $\mathcal{H}_1 = \text{span}\{|a\rangle|x\rangle\} \equiv \mathbb{C}^4 \otimes \ell^2(\mathbb{Z})$, where $a \in \{1, 2, 3, 4\}$ and $x \in \mathbb{Z}$. Namely, we have

$$\mathcal{H}_- := \text{supp}\,\mathbf{P}_-, \quad \mathbf{P}_- := \tfrac{1}{2}\big(\mathbf{I} - \mathbf{S}\big), \tag{27}$$

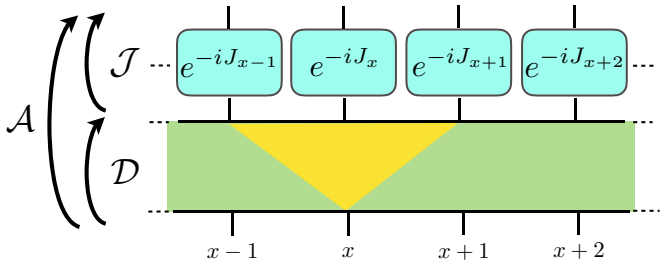

FIG. 3. The single step evolution of the FCA of Eq. (23). Each site of the lattice corresponds to a four-component fermionic field. The free evolution $\mathcal{D}$ involves the nearest neighbors while the interaction $\mathcal{J}$ is completely local.

where $\mathbf{I}$ is the identity on $\mathcal{H}_1 \otimes \mathcal{H}_1$ and $\mathbf{S}$ is the swap operator $\mathbf{S}|a_1\rangle|a_2\rangle|x_1\rangle|x_2\rangle = |a_2\rangle|a_1\rangle|x_2\rangle|x_1\rangle$, where

$$\begin{aligned} \mathcal{H}_1 \otimes \mathcal{H}_1 &= \text{span}\big\{|a_1\rangle|a_2\rangle|x_1\rangle|x_2\rangle\big\}, \\ a_1, a_2 &\in \{1, 2, 3, 4\}, \quad x_1, x_2 \in \mathbb{Z}. \end{aligned} \tag{28}$$

Let us consider the two-particle sector of $\mathcal{F}$. We have

$$\begin{aligned} \mathbf{F} \otimes \mathbf{F} = \mathbf{T} \otimes \mathbf{T} \otimes & \sum_{i,j\in\{1,4\}} |i\rangle\langle i| \otimes |j\rangle\langle j| \\ + \mathbf{T} \otimes \mathbf{T}^\dagger \otimes & \sum_{\substack{i\in\{1,4\} \\ j\in\{2,3\}}} |i\rangle\langle i| \otimes |j\rangle\langle j| \\ + \mathbf{T}^\dagger \otimes \mathbf{T} \otimes & \sum_{\substack{i\in\{2,3\} \\ j\in\{1,4\}}} |i\rangle\langle i| \otimes |j\rangle\langle j| \\ + \mathbf{T}^\dagger \otimes \mathbf{T}^\dagger \otimes & \sum_{\substack{i\in\{2,3\} \\ j\in\{2,3\}}} |i\rangle\langle i| \otimes |j\rangle\langle j|. \end{aligned} \tag{29}$$

Since we are considering local interaction, the evolution commutes with the total translation operator:

$$\mathbf{T} \otimes \mathbf{T} \otimes I|x_1\rangle|x_2\rangle|i\rangle|j\rangle = |x_1 + 1\rangle|x_2 + 1\rangle|i\rangle|j\rangle. \tag{30}$$

Therefore, it convenient to introduce the relative coordinate basis [41]

$$|x_1\rangle|x_2\rangle|i\rangle|j\rangle \mapsto |z\rangle|y\rangle|i\rangle|j\rangle, \tag{31}$$

$$y := x_1 - x_2, \quad z := x_1 + x_2 \tag{32}$$

and to Fourier transform the z coordinate, i.e.,

$$|p\rangle|y\rangle|i\rangle|j\rangle := \left(\sum_{z\in\mathbb{Z}} e^{-ipz}|z\rangle\right)|y\rangle|i\rangle|j\rangle. \tag{33}$$

In this basis, the free evolution $\mathbf{F} \otimes \mathbf{F}$ becomes

$$\begin{aligned} \mathbf{F} \otimes \mathbf{F} &= \int_\pi^\pi |p\rangle\langle p| \otimes \mathbf{F}_2(p), \\ \mathbf{F}_2(p) &:= e^{-ip}\mathbf{I} \otimes \sum_{i,j\in\{1,4\}} |i\rangle\langle i| \otimes |j\rangle\langle j| \\ &\quad + \mathbf{T} \otimes \sum_{\substack{i\in\{1,4\} \\ j\in\{2,3\}}} |i\rangle\langle i| \otimes |j\rangle\langle j| \end{aligned}$$

$$+\mathbf{T}^\dagger \otimes \sum_{\substack{i\in\{2,3\}\\ j\in\{1,4\}}} |i\rangle\langle i| \otimes |j\rangle\langle j| + e^{ip}\mathbf{I} \otimes \sum_{\substack{i\in\{2,3\}\\ j\in\{2,3\}}} |i\rangle\langle i| \otimes |j\rangle\langle j|. \tag{34}$$

Let us now consider the interaction terms of Eq. (20). Since we are considering the two-particle sector only the four-fermion interaction acts nontrivially. We notice that the free evolution of Eq. (24) does not change the relative direction of propagation of the modes. In order to have a richer phenomenology we investigate the interaction with the constant λ_1 in Eq. (19) which couples modes with different relative direction of propagation. Then, the interaction term reads as follows:

$$\begin{aligned}\mathcal{J}(\psi_{x,a}) &:= \exp\left(-i\sum_x J_x\right)\psi_{x,a}\exp\left(i\sum_x J_x\right),\\ J_x &:= \lambda O_x + \bar{\lambda} O_x^\dagger, \quad \lambda \in \mathbb{C},\\ O_x &:= \psi_{x,2}\psi_{x,3}^\dagger\psi_{x,3}\psi_{x,4}^\dagger + \psi_{x,1}\psi_{x,3}^\dagger\psi_{x,4}^\dagger\psi_{x,4}.\end{aligned} \tag{35}$$

From a straightforward computation it follows that the two-particle sector of $\mathcal{J}$ is described by the unitary operator $\mathbf{J}_2 := \mathbf{P}_-\mathbf{J}\mathbf{P}_-$, where

$$\begin{aligned}\mathbf{J} &:= \exp\left(-i\sum_x \mathbf{J}_x\right),\\ \mathbf{J}_x &:= (\lambda\mathbf{O} + \bar{\lambda}\mathbf{O}^\dagger)\otimes|x\rangle\langle x|\otimes|x\rangle\langle x|,\\ \mathbf{O} &:= |3\rangle\langle 1|\otimes|4\rangle\langle 4| + |3\rangle\langle 3|\otimes|4\rangle\langle 2|\\ &\quad + |4\rangle\langle 2|\otimes|3\rangle\langle 3| + |4\rangle\langle 4|\otimes|3\rangle\langle 1|.\end{aligned} \tag{36}$$

Since $[\mathbf{F}\otimes\mathbf{F}, \mathbf{P}_-] = [\mathbf{J}, \mathbf{P}_-] = 0$, we have that the two-particle sector of $\mathcal{A}$ is described by the operator

$$\mathbf{A}_2 := \mathbf{P}_-\left[\mathbf{J}\,(\mathbf{F}\otimes\mathbf{F})\right]\mathbf{P}_-. \tag{37}$$

Therefore, the goal of this section is to diagonalize the operator $\mathbf{A}_2$. Let us now define

$$\mathbf{Q} := \mathbf{Q}'\otimes\mathbf{I}\otimes\mathbf{I}, \tag{38}$$

$$\begin{aligned}\mathbf{Q}' := {} & |2\rangle\langle 2|\otimes|3\rangle\langle 3| + |3\rangle\langle 3|\otimes|2\rangle\langle 2|\\ & + |3\rangle\langle 3|\otimes|4\rangle\langle 4| + |4\rangle\langle 4|\otimes|3\rangle\langle 3|\\ & + |1\rangle\langle 1|\otimes|4\rangle\langle 4| + |4\rangle\langle 4|\otimes|1\rangle\langle 1|.\end{aligned} \tag{39}$$

From a straightforward computation we have $[\mathbf{A}_2, \mathbf{Q}] = 0$ and therefore we can write

$$\begin{aligned}\mathbf{A}_2 &:= \widetilde{\mathbf{A}}_2 \oplus \widetilde{\mathbf{A}}_2^\perp, \quad \widetilde{\mathbf{A}}_2, := \mathbf{Q}\mathbf{A}_2\mathbf{Q},\\ \widetilde{\mathbf{A}}_2^\perp &:= (\mathbf{I}-\mathbf{Q})\mathbf{A}_2(\mathbf{I}-\mathbf{Q}).\end{aligned} \tag{40}$$

Since $\mathbf{Q}\mathbf{J} = \mathbf{J}\mathbf{Q} = 0$, we have that $\widetilde{\mathbf{A}}_2^\perp$ is a free evolution. Therefore, we focus our analysis on the nontrivial term $\widetilde{\mathbf{A}}_2$. Let us define the vectors

$$\begin{aligned}&|e_1\rangle := |1\rangle|4\rangle, \quad |e_2\rangle := |3\rangle|2\rangle, \quad |e_3\rangle := |3\rangle|4\rangle,\\ &|e_4\rangle := |4\rangle|1\rangle, \quad |e_5\rangle := |2\rangle|3\rangle, \quad |e_6\rangle := |4\rangle|3\rangle\end{aligned} \tag{41}$$

and the Hilbert space $\widetilde{\mathcal{H}} := \mathrm{span}\{|e_i\rangle, \}$. In the basis of Eq. (41), we have

$$\lambda\mathbf{O} + \bar{\lambda}\mathbf{O}^\dagger = \begin{pmatrix}\mathbf{O}' & \mathbf{0}\\ \mathbf{0} & \mathbf{O}'\end{pmatrix}, \quad \mathbf{O}' := \begin{pmatrix}0 & 0 & -\bar{\lambda}\\ 0 & 0 & -\bar{\lambda}\\ -\lambda & -\lambda & 0\end{pmatrix}. \tag{42}$$

If we consider the total translation operator

$$\mathbf{T}_2|e_i\rangle|x_1\rangle|x_2\rangle = |e_i\rangle|x_1+1\rangle|x_2+1\rangle \tag{43}$$

it is straightforward to verify the commutation relation $[\mathbf{T}_2, \widetilde{\mathbf{A}}_2] = 0$. Therefore, it is convenient to introduce the relative coordinate basis [41]

$$|e_i\rangle|x_1\rangle|x_2\rangle \mapsto |e_i\rangle|y\rangle|z\rangle, \tag{44}$$

$$y := x_1 - x_2, \quad z := x_1 + x_2 \tag{45}$$

and to Fourier transform the z coordinate, i.e.,

$$|e_i\rangle|y\rangle|p\rangle := |e_i\rangle|y\rangle\sum_{z\in\mathbb{Z}} e^{-ipz}|z\rangle. \tag{46}$$

In this basis, the operator $\widetilde{\mathbf{A}}_2$ can be written as follows:

$$\widetilde{\mathbf{A}}_2 = \int_{-\pi}^{\pi} dp\ \widetilde{\mathbf{A}}_2(p)\otimes|p\rangle\langle p|, \tag{47}$$

$$\widetilde{\mathbf{A}}_2(p) := \widetilde{\mathbf{P}}_-\,\widetilde{\mathbf{J}}\,\widetilde{\mathbf{D}}_p\,\widetilde{\mathbf{P}}_-, \tag{48}$$

$$\widetilde{\mathbf{J}} := \exp\left[-i\begin{pmatrix}\mathbf{O}' & \mathbf{0}\\ \mathbf{0} & \mathbf{O}'\end{pmatrix}\otimes|0\rangle\langle 0|\right], \tag{49}$$

$$\widetilde{\mathbf{D}}_p := \begin{pmatrix}e^{2ip} & 0 & 0 & 0 & 0 & 0\\ 0 & e^{-2ip} & 0 & 0 & 0 & 0\\ 0 & 0 & \mathbf{T}_y^{\dagger 2} & 0 & 0 & 0\\ 0 & 0 & 0 & e^{2ip} & 0 & 0\\ 0 & 0 & 0 & 0 & e^{-2ip} & 0\\ 0 & 0 & 0 & 0 & 0 & \mathbf{T}_y^2\end{pmatrix}, \tag{50}$$

$$\widetilde{\mathbf{P}}_- := \frac{1}{2}\left[\mathbf{I}\otimes\mathbf{I} - \begin{pmatrix}\mathbf{0} & \mathbf{I}\\ \mathbf{I} & \mathbf{0}\end{pmatrix}\otimes\sum_y |-y\rangle\langle y|\right]. \tag{51}$$

Since the eigenvalues of $\mathbf{O}'$ are $0, \pm\sqrt{2}|\lambda|$ we have that $\widetilde{\mathbf{J}}$ is the identity if $\sqrt{2}|\lambda|$ is an integer multiple of 2π. Therefore, we will assume that $\sqrt{2}|\lambda| \neq 2n\pi$ $(n \in \mathbb{Z})$. Then, we can focus on the diagonalization of the (infinite-dimensional) operator $\widetilde{\mathbf{A}}_2(p)$. Let us now consider the following subspaces (see also Fig. 4):

$$\begin{aligned}\widetilde{\mathcal{H}}_a &:= \mathrm{span}\{|e_1\rangle|y\rangle - |e_4\rangle|-y\rangle, y\neq 0\},\\ \widetilde{\mathcal{H}}_b &:= \mathrm{span}\{|e_2\rangle|y\rangle - |e_5\rangle|-y\rangle, y\neq 0\},\\ \widetilde{\mathcal{H}}_c &:= \mathrm{span}\{|e_3\rangle|2y+1\rangle - |e_6\rangle|-2y-1\rangle\},\\ \widetilde{\mathcal{H}}_d &:= (\widetilde{\mathcal{H}}_a\oplus\widetilde{\mathcal{H}}_b\oplus\widetilde{\mathcal{H}}_c)^\perp.\end{aligned} \tag{52}$$

We remark that

$$\mathrm{supp}\,\widetilde{\mathbf{P}}_- = \widetilde{\mathcal{H}}_a\oplus\widetilde{\mathcal{H}}_b\oplus\widetilde{\mathcal{H}}_c\oplus\widetilde{\mathcal{H}}_d. \tag{53}$$

We are now ready to proceed with the derivation of the spectral resolution of $\widetilde{\mathbf{A}}_2(p)$. For the sake of clarity, we split the proof into several lemmas.

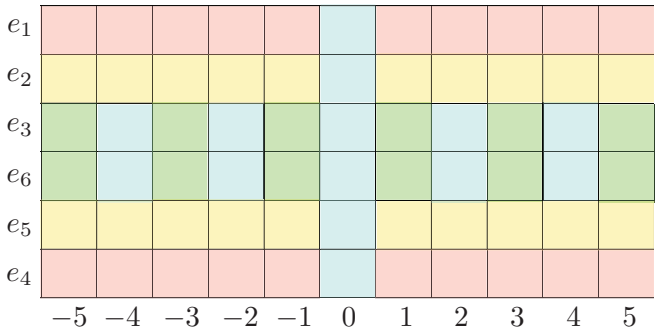

FIG. 4. Schematic representation of the decomposition of Eq. (52). On the horizontal axis we have the spatial degrees of freedom, and on the vertical axis we have the internal ones. $\widetilde{\mathcal{H}}_a$ corresponds to the red region, $\widetilde{\mathcal{H}}_b$ corresponds to the yellow region, $\widetilde{\mathcal{H}}_c$ corresponds to the green region, and $\widetilde{\mathcal{H}}_d$ corresponds to the blue region. Only states with support in $\widetilde{\mathcal{H}}_d$ are affected by the interaction.

Lemma 1. Let $\widetilde{\mathbf{A}}_2(p)$ be defined as in Eq. (48). Then we have

$$\widetilde{\mathbf{A}}_2(p) = e^{i2p}\widetilde{\mathbf{P}}_a + e^{-i2p}\widetilde{\mathbf{P}}_b + \widetilde{\mathbf{P}}_c\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_c + \widetilde{\mathbf{P}}_d\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_d \tag{54}$$

where $\widetilde{\mathbf{P}}_i$, denotes the orthogonal projector on $\widetilde{\mathcal{H}}_i$.

Proof. The subspaces $\widetilde{\mathcal{H}}_i$ in Eq. (52) are invariant subspaces of $\widetilde{\mathbf{A}}_2(p)$. One can directly verify that $\widetilde{\mathbf{P}}_a\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_a = e^{i2p}\widetilde{\mathbf{P}}_a$ and $\widetilde{\mathbf{P}}_b\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_b = e^{-i2p}\widetilde{\mathbf{P}}_b$. ■

Lemma 2. The operator $\widetilde{\mathbf{P}}_c\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_c$ has the following spectral resolution:

$$\widetilde{\mathbf{P}}_c\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_c = \int_{-\pi}^{\pi} dk\, e^{-ik}|\phi_f(k)\rangle\langle\phi_f(k)|,$$
$$|\phi_f(k)\rangle := \frac{1}{\sqrt{2}}(|e_3\rangle|k\rangle_o - |e_6\rangle|-k\rangle_o),$$
$$|k\rangle_o := \sum_{y\in\mathbb{Z}} \frac{1}{\sqrt{2\pi}} e^{-iky}|2y+1\rangle. \tag{55}$$

Proof. We have $\widetilde{\mathbf{P}}_c\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_c = \widetilde{\mathbf{P}}_c\,\widetilde{\mathbf{J}}\,\widetilde{\mathbf{D}}_p\,\widetilde{\mathbf{P}}_c$. Let us define the subspace $\ell^2(2\mathbb{Z}+1) := \mathrm{span}\{|2y+1\rangle, y\in\mathbb{Z}\} \subset \ell^2(\mathbb{Z})$ and let us denote with $\widetilde{\mathbf{P}}_{\mathrm{odd}}$ the projector on $\ell^2(2\mathbb{Z}+1)$. It is easy to verify that $\widetilde{\mathbf{P}}_c(\mathbf{I}\otimes\widetilde{\mathbf{P}}_{\mathrm{odd}}) = (\mathbf{I}\otimes\widetilde{\mathbf{P}}_{\mathrm{odd}})\widetilde{\mathbf{P}}_c = \widetilde{\mathbf{P}}_c$. Since $\widetilde{\mathbf{J}}$ is localized at the origin, we have that

$$\begin{aligned}\widetilde{\mathbf{P}}_c\,\widetilde{\mathbf{J}}\,\widetilde{\mathbf{D}}_p\,\widetilde{\mathbf{P}}_c &= \widetilde{\mathbf{P}}_c\,(\mathbf{I}\otimes\widetilde{\mathbf{P}}_{\mathrm{odd}})\,\widetilde{\mathbf{J}}\,\widetilde{\mathbf{D}}_p\,(\mathbf{I}\otimes\widetilde{\mathbf{P}}_{\mathrm{odd}})\,\widetilde{\mathbf{P}}_c\\ &= \widetilde{\mathbf{P}}_c\,(\mathbf{I}\otimes\widetilde{\mathbf{P}}_{\mathrm{odd}})\,\widetilde{\mathbf{D}}_p\,(\mathbf{I}\otimes\widetilde{\mathbf{P}}_{\mathrm{odd}})\,\widetilde{\mathbf{P}}_c\\ &= \widetilde{\mathbf{P}}_c\big(|e_3\rangle\langle e_3|\otimes\mathbf{P}_{\mathrm{odd}}\mathbf{T}_y^{\dagger 2}\mathbf{P}_{\mathrm{odd}}\big)\widetilde{\mathbf{P}}_c\\ &\quad + \widetilde{\mathbf{P}}_c\,\big(|e_6\rangle\langle e_6|\otimes\mathbf{P}_{\mathrm{odd}}\mathbf{T}_y^{2}\mathbf{P}_{\mathrm{odd}}\big)\widetilde{\mathbf{P}}_c.\end{aligned}$$

The operator $\mathbf{P}_{\mathrm{odd}}\mathbf{T}_y^2\mathbf{P}_{\mathrm{odd}}$ is easily diagonalized as follows:

$$\mathbf{P}_{\mathrm{odd}}\mathbf{T}_y^2\mathbf{P}_{\mathrm{odd}} = \int_{-\pi}^{\pi} dk\, e^{-ik}|k\rangle_o\langle k|_o.$$

Then we have

$$|e_3\rangle\langle e_3|\otimes\mathbf{P}_{\mathrm{odd}}\mathbf{T}_y^{\dagger 2}\mathbf{P}_{\mathrm{odd}} + |e_6\rangle\langle e_6|\otimes\mathbf{P}_{\mathrm{odd}}\mathbf{T}_y^{2}\mathbf{P}_{\mathrm{odd}}$$
$$= \int_{-\pi}^{\pi} dk\, e^{-ik}(|e_3\rangle\langle e_3|\otimes|k\rangle_o\langle k|_o + |e_6\rangle\langle e_6|\otimes|-k\rangle_o\langle -k|_o).$$

Since $\widetilde{\mathbf{P}}_c|e_3\rangle|k\rangle_o = -\widetilde{\mathbf{P}}_c|e_6\rangle|-k\rangle_o = 1/\sqrt{2}|\phi_f(k)\rangle$ we have the thesis. ■

Lemma 3. We have the following spectral resolutions.
(1) $\sqrt{2}|\lambda| \neq n\pi$ and $2p \neq n'\pi$ with $n, n' \in \mathbb{Z}$:

$$\widetilde{\mathbf{P}}_d\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_d = \int_{-\pi}^{\pi} dk\, e^{-ik}|\phi_s(k)\rangle\langle\phi_s(k)|. \tag{56}$$

(2) $\sqrt{2}|\lambda| \neq n\pi$ and $2p = n'\pi$ with $n, n' \in \mathbb{Z}$:

$$\widetilde{\mathbf{P}}_d\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_d = \int_{-\pi}^{\pi} dk\, e^{-ik}|\phi_s(k)\rangle\langle\phi_s(k)| + (-1)^{n'}|\phi_{b0}\rangle\langle\phi_{b0}|. \tag{57}$$

(3) $\sqrt{2}|\lambda| = (2n+1)\pi$ with $n \in \mathbb{Z}$:

$$\widetilde{\mathbf{P}}_d\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_d = \int_{-\pi}^{\pi} dk\, e^{-ik}|\phi_s(k)\rangle\langle\phi_s(k)| + |\phi_{b-}\rangle\langle\phi_{b-}| - |\phi_{b+}\rangle\langle\phi_{b+}|. \tag{58}$$

Here we defined

$$\begin{aligned}N_k|\phi_s(k)\rangle :=& \sum_{y\geqslant 1}\overline{c_k}e^{-iyk}(|e_3\rangle|2y\rangle - |e_6\rangle|-2y\rangle)\\ &+ \sum_{y\leqslant 0} c_k e^{-iyk}(|e_3\rangle|2y\rangle - |e_6\rangle|-2y\rangle)\\ &+ |\psi_0\rangle|0\rangle,\end{aligned} \tag{59}$$

$$|\psi_0\rangle := d_k(|e_1\rangle - |e_4\rangle) - \overline{d_{-k}}(|e_2\rangle - |e_5\rangle), \tag{60}$$

$$|\phi_{b0}\rangle := \frac{1}{2}(|e_1\rangle - |e_4\rangle - |e_2\rangle + |e_5\rangle)|0\rangle, \tag{61}$$

$$|\phi_{b-}\rangle := \frac{1}{2}[e^{-ip}(|e_1\rangle - |e_4\rangle) - e^{ip}(|e_2\rangle - |e_5\rangle)]|0\rangle, \tag{62}$$

$$|\phi_{b+}\rangle := \frac{1}{2}[e^{-ip}(|e_1\rangle - |e_4\rangle) + e^{ip}(|e_2\rangle - |e_5\rangle)]|0\rangle, \tag{63}$$

$$c_k := \cos(\sqrt{2}|\lambda|)[e^{-ik} - \cos(2p)] + [e^{ik} - \cos(2p)], \tag{64}$$

$$d_k := \frac{i\overline{\lambda}\sin(\sqrt{2}|\lambda|)}{\sqrt{2}|\lambda|}(e^{-ik} - e^{-i2p}), \tag{65}$$

and N_k is a suitable normalization constant such that $\langle\phi_s(k)|\phi_s(k')\rangle = \delta(k-k')$.

Proof. Let us consider the first case. One can verify by direct computation that $\overline{N_k}N_{k'}\langle\phi_s(k)|\phi_s(k')\rangle \propto \delta(k-k')$ and that $N_k|\phi_s(k)\rangle$ are improper eigenstates of $\widetilde{\mathbf{P}}_d\widetilde{\mathbf{A}}_2(p)\widetilde{\mathbf{P}}_d$ with eigenvalue e^{-ik}. Similarly, one also verifies (in the appropriate cases) that $|\phi_{b0}\rangle$, $|\phi_{b+}\rangle$, and $|\phi_{b-}\rangle$ are also eigenstates. One then has to verify the completeness relation $\int_{-\pi}^{\pi}|\phi_s(k)\rangle\langle\phi_s(k)| = \widetilde{\mathbf{P}}_d$ (and the completeness of the other spectral resolutions). This will be done in Appendix A. ■

We can combine the statements of Lemmas 1–3 into a single proposition which summarizes the results of this section.

Proposition 1. The unitary operator $\mathbf{A}_2$, defined in Eq. (37), describes the single step evolution of the two-particle sector of the FCA $\mathcal{A}$ of Eq. (23). From Eq. (40) we have the following decomposition:

$$\mathbf{A}_2 = \widetilde{\mathbf{A}}_2 \oplus \widetilde{\mathbf{A}}_2^{\perp}. \tag{66}$$

The operator $\widetilde{\mathbf{A}}_2^{\perp}$ acts as the free evolution and the operator $\mathbf{A}_2$ has the following spectral resolution:

$$\widetilde{\mathbf{A}}_2 = \int_{-\pi}^{\pi} dp\ \widetilde{\mathbf{A}}_2(p) \otimes |p\rangle\langle p|, \tag{67}$$

$$\widetilde{\mathbf{A}}_2(p) = e^{i2p}\widetilde{\mathbf{P}}_a + e^{-i2p}\widetilde{\mathbf{P}}_b + \widetilde{\mathbf{B}} + \int_{-\pi}^{\pi} dk\, e^{-ik}[|\phi_f(k)\rangle\langle\phi_f(k)| + |\phi_s(k)\rangle\langle\phi_s(k)|],$$

$$\widetilde{\mathbf{B}} \coloneqq \begin{cases} (-1)^{n'}|\phi_{b0}\rangle\langle\phi_{b0}| & \sqrt{2}|\lambda| \neq (n+1)\pi \\ & \text{and } 2p = n'\pi, \\ |\phi_{b-}\rangle\langle\phi_{b-}| - |\phi_{b+}\rangle\langle\phi_{b+}| & \sqrt{2}|\lambda| = (n+1)\pi \\ 0 & \text{otherwise,} \end{cases} \tag{68}$$

where we remind the reader that $|p\rangle$ are the (improper) eigenstates of the total momentum and that $\widetilde{\mathbf{A}}_2(p)$ acts on the relative coordinate and the internal degrees of freedom.

IV. CONCLUSIONS

In this paper we have studied the two-particle sector of an interacting FCA. The free evolution is modeled after the massless Dirac quantum walk [20] while the interaction is quartic, local, and number preserving. The interaction has been chosen among the ones with these properties which are invariant under the isotropy group of the Weyl cellular automata. Those interactions have been classified with the help of our in-house code employing the symbolic mathematics module SYMPY. The code is available on GitHub and the result of the classification is given in Eq. (19).

For the specific case considered, the dynamics of the two-particle sector, for a fixed value of the total momentum, can be described as a single massless particle (the relative position) moving on a one-dimensional lattice with a potential which is localized at the origin and that interacts with the internal degrees of freedom. The spectral resolution of the evolution operator provides a complete account of the dynamics. Referring to Proposition 1 we have the following.

(i) The projectors $\widetilde{\mathbf{P}}_a$ and $\widetilde{\mathbf{P}}_b$ project on subspaces which are orthogonal to the support of the interaction term and on which the free evolution acts only as total translation of the center of mass. States in these subspaces describe particles that experience no relative motion and no interaction.

(ii) The (improper) eigenstates $|\phi_f(k)\rangle$ describe free particles that experience relative motion but do not feel the presence of the interaction because they never happen to be in the same site (in the relative coordinate they stay confined on the odd sites while the interaction is localized at zero).

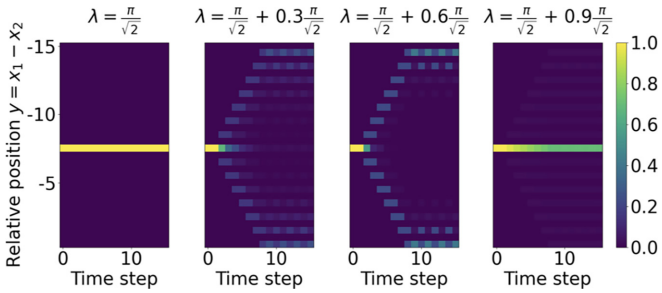

FIG. 5. Numerical simulation of $\widetilde{\mathbf{A}}_2(p)$ with $p = \pi/4$ and $\lambda \in (\pi/\sqrt{2}, 2\pi/\sqrt{2})$. On the x axis we report the simulation time step, while on the y axis we report the relative position of the two particles. The probability of finding the particles at a certain relative position after measuring over the internal degrees of freedom is reported in color scale. Bound states are observed around values $\lambda = n\pi/\sqrt{2}$, $n \in \mathbb{Z}$, while scattering states arise for values in between two subsequent integer multiples of $\pi/\sqrt{2}$. The initial state is $|\phi_{b+}\rangle = \frac{1}{2}[e^{-ip}(|e_1\rangle - |e_4\rangle) + e^{+ip}(|e_2\rangle - |e_5\rangle)]|0\rangle$.

(iii) The (improper) eigenstates $|\phi_s(k)\rangle$ describe particles that move relative to each other and that can interact. These states describe the scattering processes.

(iv) The states $|\phi_{b0}\rangle$, $|\phi_{b+}\rangle$, and $|\phi_{b-}\rangle$ describe bound states (see Fig. 5). The latter are perfectly localized and they occur only for some critical value of the total momentum p or some critical value of the coupling constant λ.

The origin of this phenomenon can be traced back to the time discreteness of the QCA model. When we exponentiate an Hamiltonian operator H, the resulting unitary operator $\exp(-iH)$ can have degeneracies because of the periodicity of the exponential function. This is what happens to the free evolution for $2p = n\pi$ and to the interacting term for $\sqrt{2}|\lambda| = (2n+1)\pi$. At those critical values we find common eigenstates of the free evolution $\widetilde{\mathbf{D}}_p$ and of the interaction $\widetilde{\mathbf{J}}$. Further studies are planned to determine whether the one-particle and two-particle solutions provide sufficient information to solve the dynamics in all number sectors. This would open the route for a statistical analysis of the model, in order to determine whether it admits of phase transitions or other critical phenomena. Another interesting development consists in the study of bound states as virtual particles and their effective interactions with other stationary states.

The codes used in this paper to derive the most general interaction in our setting and to simulate the interacting QW studied are publicly available on the GitHub repository [42].

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APPENDIX A: COMPLETENESS OF THE SOLUTIONS

Let us now prove the completeness of the solution set found in the previous section. A vector $|\chi\rangle$ in $\widetilde{\mathcal{H}}_d$ can be written as

follows:

$$|\chi\rangle = |\chi_0\rangle|0\rangle + \sum_y \overline{c_{3,y}}(|e_3\rangle|2y\rangle - |e_6\rangle|-2y\rangle),$$

$$|\chi_0\rangle := \overline{c_{1,0}}(|e_1\rangle - |e_4\rangle) + \overline{c_{2,0}}(|e_2\rangle - |e_5\rangle). \tag{A1}$$

From Eq. (59) we have that

$$\begin{aligned}
\langle\chi|\phi_s(k)\rangle &= 2f(k),\\
f(k) &= c_{1,0}d_k + c_{2,0}\overline{d_{-k}} + \sum_{y\leqslant 0} c_{3,y}c_k e^{-iyk}\\
&\quad + \sum_{y\geqslant 1} c_{3,y}\overline{c_k}e^{-iyk}\\
&= \sum_{y\leqslant -1}(\gamma c_{3,y-1} - \epsilon c_{3,y} + c_{3,y+1})e^{-iyk}\\
&\quad + \gamma c_{3,-1} - \epsilon c_{3,0} + \sigma e^{-i2p}c_{1,0} + \sigma e^{i2p}c_{2,0}\\
&\quad + \delta c_{3,1}\\
&\quad + (\gamma c_{3,0} - \sigma c_{1,0} - \sigma c_{2,0} - \epsilon c_{3,1} + \delta c_{3,2})e^{-ik}\\
&\quad + \sum_{y\geqslant 2}(c_{3,y-1} - \epsilon c_{3,y} + \gamma c_{3,y+1})e^{-iyk},\\
\gamma &:= \cos(\sqrt{2}|\lambda|), \quad \epsilon := \cos(2p)(\gamma+1),\\
\sigma &:= -\frac{i\bar{\lambda}\sin(\sqrt{2}|\lambda|)}{\sqrt{2}|\lambda|}.
\end{aligned} \tag{A2}$$

Therefore, the condition $\langle\chi|\phi_s(k)\rangle = 0$ is equivalent to $f(k) = 0$ for any k. Since $f(k)$ is a Fourier series, the condition $f(k) = 0$ for any k implies the following system of equations:

$$\begin{aligned}
0 &= \gamma c_{3,y-1} - \epsilon c_{3,y} + c_{3,y+1} \quad \text{for } y \leqslant -1,\\
0 &= \gamma c_{3,-1} - \epsilon c_{3,0} + \sigma e^{-i2p}c_{1,0}\\
&\quad + \sigma e^{i2p}c_{2,0} + \delta c_{3,1},\\
0 &= \gamma c_{3,0} - \sigma c_{1,0} - \sigma c_{2,0} - \epsilon c_{3,1} + \delta c_{3,2},\\
0 &= c_{3,y-1} - \epsilon c_{3,y} + \gamma c_{3,y+1} \quad \text{for } y \geqslant 2.
\end{aligned} \tag{A3}$$

Equation (A3) can be conveniently rewritten as follows:

$$0 = \gamma x_{n-1} - \epsilon x_n + x_{n+1} \quad \text{for } n \leqslant -1, \tag{A4}$$

$$\begin{aligned}
0 &= \gamma x_{-1} - \epsilon x_0 + \sigma e^{-i2p}x_1\\
&\quad + \sigma e^{i2p}x_2 + \gamma x_3,
\end{aligned} \tag{A5}$$

$$0 = \gamma x_0 - \sigma x_1 - \sigma x_2 - \epsilon x_3 + \gamma x_4, \tag{A6}$$

$$0 = x_{n-1} - \epsilon x_n + \gamma x_{n+1} \quad \text{for } n \geqslant 4, \tag{A7}$$

$$x_n = \begin{cases} c_{3,n} & n \leqslant 0\\ c_{1,0} & n = 1\\ c_{2,0} & n = 2\\ c_{3,n-2} & n \geqslant 3 \end{cases}. \tag{A8}$$

If $2\sqrt{2}|\lambda| = n\pi$ then we have $\gamma = 0$ and Eqs. (A4) to (A7) simplify as follows:

$$0 = -\epsilon x_n + x_{n+1} \quad \text{for } n \leqslant -1, \tag{A9}$$

$$0 = -\epsilon x_0 + \sigma e^{-i2p}x_1 + \sigma e^{i2p}x_2, \tag{A10}$$

$$0 = -\sigma x_1 - \sigma x_2 - \epsilon x_3, \tag{A11}$$

$$0 = x_{n-1} - \epsilon x_n \quad \text{for } n \geqslant 4. \tag{A12}$$

If also $\epsilon = 0$ then Eqs. (A9) and (A12) imply $x_n = 0$ for $n \geqslant 3$ and $n \leqslant 0$. On the other hand, if $\epsilon \neq 0$ the linear recurrence relations (A9) and (A12) have the solutions

$$\begin{aligned}
x_{-n} &= \epsilon^{-n}x_0 \quad \text{for } n \geqslant 1,\\
x_{n+3} &= \epsilon^{-n}x_3 \quad \text{for } n \geqslant 1.
\end{aligned} \tag{A13}$$

However, $\gamma = 0$ implies that $|\epsilon| = |\cos(2p)| \leqslant 1$ and the convergence of $\sum_n |x_n|^2$ implies that $x_0 = x_3 = 0$. We then conclude that $x_n = 0$ for $n \geqslant 3$ and $n \leqslant 0$.

Let us now suppose that $2\sqrt{2}|\lambda| \neq n\pi$, which implies $\gamma \neq 0$. The linear recurrence relations (A3) and (A7) can be rewritten as follows:

$$x_{-n-1} - \frac{\epsilon}{\gamma}x_{-n} + \frac{1}{\gamma}x_{-n+1} = 0 \quad \text{for } n \geqslant 1, \tag{A14}$$

$$x_{n+1} - \frac{\epsilon}{\gamma}x_n + \frac{1}{\gamma}x_{n-1} = 0 \quad \text{for } n \geqslant 4. \tag{A15}$$

If $\epsilon = 0$ we have

$$x_{-2n} = \left(-\frac{1}{\gamma}\right)^n x_0 \quad \text{for } n \geqslant 1, \tag{A16}$$

$$x_{2n+1} = \left(-\frac{1}{\gamma}\right)^n x_3 \quad \text{for } n \geqslant 1. \tag{A17}$$

Therefore, the convergence of $\sum_n |x_n|^2$ implies that $x_n = 0$ for $n \geqslant 3$ and $n \leqslant 0$. Let us now suppose that $\gamma, \epsilon \neq 0$. The characteristic equations of the recurrence relations (A14) and (A17) are the same and have the roots

$$r_\pm = \frac{\epsilon \pm \sqrt{\epsilon^2 - 4\gamma}}{2\gamma}. \tag{A18}$$

If $\epsilon^2 - 4\gamma = 0$ then $r_+ = r_- = r = \frac{\epsilon}{2\gamma}$ and

$$x_{-n} = (a + bn)r^n \quad \text{for } n \geqslant 0, \tag{A19}$$

$$x_{n+2} = (a' + b'n)r^n \quad \text{for } n \geqslant 1 \tag{A20}$$

for some coefficients a, a', b, and b'. Since $|r| = \frac{|\epsilon|}{2|\gamma|} = \frac{2}{|\epsilon|} \geqslant 1$ the convergence of $\sum_n |x_n|^2$ implies that $x_n = 0$ for $n \geqslant 3$ and $n \leqslant 0$. If $\epsilon^2 \geqslant 4\gamma \neq 0$ then r_+ and r_- are distinct and the solution of the recurrence relation is

$$x_{-n} = ar_-^n + br_+^n \quad \text{for } n \geqslant 0, \tag{A21}$$

$$x_{n+2} = a'r_-^n + b'r_+^n \quad \text{for } n \geqslant 1 \tag{A22}$$

for some coefficients a, a', b, and b'. One can verify (see Appendix B) that $|r_\pm| \geqslant 1$ and the convergence of $\sum_n |x_n|^2$ implies that $x_n = 0$ for $n \geqslant 3$ and $n \leqslant 0$. We have then proved that Eqs. (A4) and (A7) imply that $x_n = 0$ for $n \geqslant 3$ and $n \leqslant 0$. Then, Eqs. (A10) and (A11) become

$$\begin{aligned}
0 &= \sigma e^{-i2p}x_1 + \sigma e^{i2p}x_2,\\
0 &= -\sigma x_1 - \sigma x_2.
\end{aligned} \tag{A23}$$

If $\sqrt{2}|\lambda| \neq n\pi \iff \sigma \neq 0$ and $\sin(2p) \neq 0$ Eq. (A23) implies $x_1 = x_2 = 0$. If $\sigma \neq 0$ and $\sin(2p) = 0$ we have the solution $x_1 = -x_2$ and the orthogonality with $|\phi_{b0}\rangle$ gives $x_1 = x_2 = 0$. Similarly, if $\sigma = 0$ the orthogonality with $|\phi_{b1}\rangle$ and $|\phi_{b2}\rangle$ implies $x_1 = x_2 = 0$.

APPENDIX B: STUDY OF $|r_\pm|$

We will prove that $|r_\pm| > 1$ by considering three cases.

1. $\epsilon^2 - 4\gamma > 0$ and $\gamma > 0$

If $\epsilon^2 - 4\gamma > 0$ then $r_\pm \in \mathbb{R}$. If $\gamma > 0$ we have

$$|r_\pm| = \frac{|\epsilon \pm \sqrt{\epsilon^2 - 4\gamma}|}{2\gamma} \geqslant \frac{|\epsilon| - \sqrt{\epsilon^2 - 4\gamma}}{2\gamma}.$$

Since $\epsilon^2 - 4\gamma > 0$ and $|\gamma| \leqslant 1$ imply $|\epsilon| - 2|\gamma| > 0$ we have

$$\frac{|\epsilon| - \sqrt{\epsilon^2 - 4\gamma}}{2\gamma} \geqslant 1 \iff |\epsilon| - 2\gamma \geqslant \sqrt{\epsilon^2 - 4\gamma} \iff$$
$$(|\epsilon| - 2\gamma)^2 \geqslant \epsilon^2 \iff \gamma - |\epsilon| \geqslant -1 \iff$$
$$\gamma - |\cos(2p)(1+\gamma)| \geqslant -1 \iff$$
$$[1 - |\cos(2p)|]\gamma - |\cos(2p)| \geqslant -1,$$

which proves that $|r_\pm| \geqslant 1$ for $\gamma > 0$.

2. $\epsilon^2 - 4\gamma > 0$ and $\gamma < 0$

If $\epsilon^2 - 4\gamma > 0$ then $r_\pm \in \mathbb{R}$. If $\gamma < 0$ we have

$$|r_\pm| = \frac{|\epsilon \pm \sqrt{\epsilon^2 - 4\gamma}|}{2\gamma} \geqslant \frac{\sqrt{\epsilon^2 + 4|\gamma|} - |\epsilon|}{2|\gamma|}.$$

Then we have

$$\frac{\sqrt{\epsilon^2 + 4|\gamma|} - |\epsilon|}{2|\gamma|} \geqslant 1 \iff \sqrt{\epsilon^2 + 4|\gamma|} \geqslant 2|\gamma| + |\epsilon| \iff$$
$$\epsilon^2 + 4|\gamma \geqslant (2|\gamma| + |\epsilon|)^2 \iff 1 \geqslant |\gamma| + |\epsilon| \iff$$
$$1 \geqslant |\gamma| + |\cos(2p)(1 - |\gamma|)| \iff$$
$$1 - |\cos(2p)| \geqslant [1 - |\cos(2p)|]|\gamma| \iff 1 \geqslant |\gamma|,$$

which proves that $|r_\pm| \geqslant 1$ for $\gamma < 0$.

3. $\epsilon^2 - 4\gamma < 0$

If $\epsilon^2 - 4\gamma < 0$ then

$$r_\pm = \frac{\epsilon \pm i\sqrt{4\gamma - \epsilon^2}}{2\gamma},$$

which implies $|r_\pm|^2 = \frac{1}{\gamma} \geqslant 1$.

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[39] Given two metric spaces (M_1, d_1) and (M_2, d_2), with d_1 and d_2 the metrics of the two spaces, a map $f : (M_1, d_1) \to (M_2, d_2)$ is a quasi-isometry [43] if there exist constants $A \geqslant 1$ and $B, C \geqslant 0$, such that $\forall g_1, g_2 \in M_1$, and one has $d_1(g_1, g_2)/A - B \leqslant d_2(f(g_1), f(g_2)) \leqslant A d_1(g_1, g_2) + B$ and $\forall m \in M_2$ if there exists $g \in M_1$ such that $d_2(f(g), m) \leqslant C$. Intuitively, if there exists a quasi-isometry between (M_1, d_1) and (M_2, d_2), then the large-scale geometries of the two spaces are the same.

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[41] We notice that only the pairs (y, z) with y and z both even or both odd correspond to integers x_1 and x_2. However, it is convenient to consider the extended Hilbert space in which y and z run free.

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