Clifford algebra from quantum automata and unitary Wilson fermions

Pablo Arnault*

Université Paris-Saclay, CNRS, ENS Paris-Saclay, INRIA, Laboratoire Méthodes Formelles, 91190 Gif-sur-Yvette, France

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We introduce a spacetime discretization of the Dirac equation that has the form of a quantum automaton and that is invariant upon changing the representation of the Clifford algebra, like the Dirac equation itself. Our derivation follows Dirac's original one: We required that the square of the discrete Dirac scheme be what we define as an acceptable discretization of the Klein-Gordon equation. In contrast to standard lattice gauge theory in discrete time, in which unitarity needs to be proven, we show that the quantum automaton delivers naturally unitary Wilson fermions for any choice of Wilson's parameter.

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I. INTRODUCTION

The Dirac equation (DE) is the law of motion of relativistic quantum particles of matter (more precisely, of so-called fermionic particles) and is one of the main equations of the standard model of particle physics. The gamma matrices are objects needed to write down the DE. These gamma matrices have to satisfy the so-called Clifford algebra. Any family of matrices that satisfy the Clifford algebra is a good candidate to write down the DE; more precisely, the DE is invariant upon changing the Clifford-algebra representation. This symmetry is fundamental: The physics is captured by the Clifford algebra, and not by a single, particular family of gamma matrices chosen. Moreover, the Clifford algebra is at the grounding of modern geometric algebra [1], which shows its fundamental character beyond the DE, for understanding the geometry of our world.

It is well known that numerically simulating real-time dynamics of quantum multiparticle systems is exponentially hard and that quantum computers could overcome this difficulty. The DE is a central ingredient of these quantum multiparticle systems in the relativistic regime. In order to perform simulations involving the DE, one starts by discretizing it on a spacetime grid [2,3]. However, if one does so without care, one breaks certain symmetries satisfied by the DE. Now, discrete-time quantum walks (DQWs) are quantum transport schemes in discrete spacetime that have been the subject of much attention in the last 30 years, in particular, because of their success as discretizations of the DE that preserve various of its symmetries [4–6], also when coupled to the fundamental force fields of nature [7–14]. There are two main such symmetries that DQWs preserve: The first is unitarity; the second, which is actually rather a property, is relativistic locality, i.e., the group velocity in a vacuum cannot overcome the speed of light. We call a DQW corresponding to a discretization of the DE that exhibits the two aforementioned properties a Dirac DQW.

To our knowledge, no existing Dirac DQW has yet managed to preserve the invariance of the DE upon changing the Clifford-algebra representation. More precisely, the representation chosen when discretizing the DE with a Dirac DQW is actually always the same, e.g., in $1+1$ dimensions, the first alpha matrix always equals the third Pauli matrix. If one chooses initially a different representation, one will need a different discretization method. So, not only the structure of the resulting discretization but also the method used to discretize the equation depend on the Clifford-algebra representation, which is strongly unsatisfying.

In this paper, we give a solution to this issue, by introducing a Dirac-DQW-based discretization method of the DE that can be carried out whatever the Clifford-algebra representation. More precisely, we make possible the emergence of the Clifford algebra out of the operators defining the Dirac DQW. This is achieved by choosing such operators that are appropriate but still independent of any choice of basis; they only need to satisfy the above-mentioned Clifford algebra. This Clifford algebra is obtained, following Dirac's own procedure in continuous spacetime, by requiring that the Dirac DQW squares a spacetime-discretized version of the Klein-Gordon equation that we consider valid, i.e., it must not only deliver the correct Klein-Gordon equation in the continuum limit but also (i) be applicable to scalar state sequences *at the discrete level* and (ii) satisfy an extra condition, namely, the vanishing of the crossed term *at the discrete level*. We then show that DQWs also contain, "naturally" (provided we make certain appropriate choices), a Wilson term that allows fermion doubling to be avoided, which is well known in lattice gauge theory (LGT). Unitarity is maintained at each step of the derivation, and this is the case *for any choice* $r \in \mathbb{R}$ *of Wilson's parameter*.

II. DISCRETE-TIME QUANTUM WALKS

A DQW is a unitary automaton with an ultralocal evolution operator. The system is called a *walker*, and its state at time $j \in \mathbb{N}$ is given by a sequence $\Psi_j : (j,p) \mapsto \Psi_{j,p}$ defined over a lattice with sites labeled by $p \in \mathbb{Z}$; the lattice

*pablo.arnault@inria.fr

is considered one dimensional (1D) for simplicity. The dynamics of this system is called a *walk*, written $\Psi_{j+1} = \mathcal{U}\Psi_j$, where $\mathcal{U}$ is the unitary one-step evolution *walk operator*. That $\mathcal{U}$ is *ultralocal* means, by definition, that the internal state $\Psi_{j+1,p}$ solely depends on internal states $\Psi_{j,p'}$ that belong to a bounded spatial-lattice neighborhood around p. In the context of automata, ultralocality of $\mathcal{U}$ is often implicit. In quantum computation it is frequent that $\mathcal{U}$ is not ultralocal: This can be either because we purposely apply, in discrete time, a gate which is nonlocal [15] or because we are in continuous time and evolve a system via a nearest-neighbors Hamiltonian which yields approximate but not exact ultralocality via Lieb-Robinson bounds [16].

To specify the nature of Ψ_j, it is useful to invoke Meyer's no-go result [5,17]: No nontrivial ultralocal unitary automaton with a one-step evolution operator that is homogeneous in space (i.e., translationally invariant) can have a scalar walker; the minimum number of internal components for $\Psi_{j,p}$ is thus 2. Hence we consider $\Psi_{j,p} \in \mathscr{H}_2$, a complex Hilbert space of dimension 2. In a formal parallel with classical random walks [18], in which a coin is tossed to determine the direction taken by the walker, the internal state $\Psi_{j,p}$ is called the *coin state*, and $\mathscr{H}_2$ is called the *coin space*.

III. TRANSPORT COIN OPERATORS OF A DQW

Consider the DQW defined initially,

$$\Psi_{j+1} = \mathcal{U}\Psi_j. \tag{1}$$

The one-step evolution operator $\mathcal{U}$ can be given under a multiplicative [19,20] or an additive form [5,6]. We here give $\mathcal{U}$ under the generic additive form $\mathcal{U} := W_{-1}\mathcal{T}_1^{-1} + W_1\mathcal{T}_1 + W_0$. In this equation, (i) $\mathcal{T}_1$ is the translation operator by one lattice site in the direction of growing p's [that is, $(\mathcal{T}_1\Psi)_{j,p} := \Psi_{j,p-1}$], and (ii) the W_i's, $i = -1, 0, 1$, are operators acting solely on the coin space, which we call *jump coin operators*. While one may view the W_i's as 2×2 complex matrices, viewing them abstractly is actually the purpose of this paper, and *we will not introduce any basis of* $\mathscr{H}_2$. The translation operator is by construction related to the momentum operator, $\mathcal{K}$, via $\mathcal{T}_1 = e^{-ia\mathcal{K}}$, where $a \in \mathbb{R}^{+,*}$ will be identified further on with the spatial-lattice spacing. In Appendix A, we derive the constraints that the unitarity of $\mathcal{U}$ imposes on the W_i's [5,6].

We define the following coin operators, which we call *transport coin operators*:

$$B := W_1 - W_{-1}, \tag{2a}$$

$$V := W_1 + W_{-1}, \tag{2b}$$

$$M := \sum_{i=-1,0,1} W_i = V + W_0. \tag{2c}$$

In terms of these operators, $\mathcal{U}$ reads $\mathcal{U} = \frac{1}{2}(V - B)\mathcal{T}_1^{-1} + \frac{1}{2}(V + B)\mathcal{T}_1 + M - V$. In Appendix A, we translate on the transport coin operators the constraints imposed on the jump coin operators by the unitarity of $\mathcal{U}$.

IV. LOCAL HAMILTONIAN OF A DQW

From the one-step dynamics $\Psi_{j+1} = \mathcal{U}\Psi_j$, one can conceive a dynamics $i(\Psi_{j+1} - \Psi_{j-1})/2 = \mathcal{H}\Psi_j$ determined by the Hermitian operator $\mathcal{H} := \frac{i}{2}(\mathcal{U} - \mathcal{U}^\dagger)$, which is (ultra)local since $\mathcal{U}$ is ultralocal, and that we call the *local Hamiltonian of the DQW*. This dynamics is "two step," meaning that while the one-step dynamics takes as the initial condition $\Psi_{j=0}$, the two-step one takes as the initial condition both $\Psi_{j=0}$ and $\Psi_{j=1}$. The two-step dynamics is equivalent to the one-step one provided that $\Psi_1 = \mathcal{U}\Psi_0$. That the Hamiltonian $\mathcal{H}$ is (ultra)local is in contrast with the case of the well-known effective Hamiltonian of the DQW. Note that both Hamiltonians are related by a proportionality constant in Fourier space [21].

The operator $\mathcal{H}$ can be written in terms of the transport coin operators as

$$\mathcal{H} = \mathcal{H}'_Q := A^1(-i\mathcal{D}_1) + \frac{r}{2}Q(-\mathcal{L}) + \epsilon m A^0, \tag{3}$$

where $m \in \mathbb{R}^+$ and $r \in \mathbb{R}$ are two parameters that we force to appear (we also force ϵ to appear in ϵm). In Eq. (3), we have introduced the following: (i) operators acting on the position space solely, $\mathcal{D}_1 := \frac{1}{2}(\mathcal{T}_1^{-1} - \mathcal{T}_1)$ and $\mathcal{L} := \mathcal{T}_1^{-1} + \mathcal{T}_1 - 2$, and (ii) coin operators made out of the transport coin operators, $A^1 := (B + B^\dagger)/2$, $Q := -\frac{i}{r}(V - V^\dagger)/2$, and $A^0 := \frac{i}{\epsilon m}(M - M^\dagger)/2$. We have used the notation $\mathcal{H} = \mathcal{H}'_Q$ because we are going to consider both the case in which $Q = 0$ and the case in which $Q \neq 0$.

V. DIRAC-CONTINUUM-LIMIT REQUIREMENT

The two-step dynamics can be written

$$i(\mathcal{D}_0\Psi)_j = \mathcal{H}\Psi_j, \tag{4}$$

where $\mathcal{D}_0 := (\mathcal{T}_0^{-1} - \mathcal{T}_0)/2$, with $\mathcal{T}_0$ being the shift by one lattice site forward in time, i.e., $(\mathcal{T}_0\Psi)_j := \Psi_{j-1}$. We wish that the two-step dynamics deliver the $(1 + 1)$D DE in the continuum limit. In order to take the continuum limit, we introduce continuous time and space coordinates t and x, as well as a function of these continuous coordinates, $\Psi(\cdot, \cdot) : (t, x) \mapsto \Psi(t, x)$, which is as smooth as wished and which coincides at coordinates $(t_j := j\epsilon, x_p := pa)$ with the "value" taken by the coin state at point (j, p), that is, $\Psi(t_j, x_p) := \Psi_{j,p}$. We then consider the ballistic scaling $\epsilon = a$ [22] and Taylor-expand the two-step dynamics in time and space around the point (t_j, x_p), at second order in ϵ.

For the continuum limit of the two-step dynamics, Eq. (4) [divide Eq. (4) by ϵ and let $\epsilon \to 0$ after the Taylor expansion at second order], to coincide with the $(1 + 1)$D DE, it is sufficient that the two following *Dirac-continuum-limit constraints* be satisfied: $A^1 := \frac{B+B^\dagger}{2} \underset{\epsilon\to 0}{\sim} \alpha^1$ and $\epsilon m A^0 := i\frac{M-M^\dagger}{2} \underset{\epsilon\to 0}{\sim} \epsilon m\alpha^0$, where α^1 and α^0 must satisfy $(\alpha^0)^2 = (\alpha^1)^2 = 1$ and $\alpha^0\alpha^1 + \alpha^1\alpha^0 = 0$, in order for them to correspond to the well-known α operators of the DE.

Note that no continuum-limit constraint is imposed on Q and thus neither is any imposed on V (apart from Q not scaling as ϵ^δ with $\delta \leqslant -1$, i.e., we must have $\delta > -1$), because as $\epsilon \to 0$, we have that $\mathcal{L} \sim \epsilon^2\partial_x^2$ while $\mathcal{D}_1 \sim \epsilon\partial_x$, so that the term $\frac{r}{2}Q(-\mathcal{L})$ in Eq. (3) vanishes in the continuum (again, provided $\delta > -1$); we call this term the *Wilson Q term*. The Wilson Q term can be chosen to be nonvanishing, and the scheme still delivers the DE. This observation will be useful further on, but for now let us consider that $Q = 0$. At this

point, one may be tempted to make the trivial choice $V = 0$ to obtain $Q = 0$, but this is unlikely to be possible due to the unitarity constraints (see Appendix A). The constraint we have in order to obtain $Q = 0$ is $V = V^\dagger$. We will see below what choice we finally make for V.

VI. KLEIN-GORDON-SQUARE REQUIREMENT AND CLIFFORD ALGEBRA FROM QUANTUM AUTOMATA

Squaring the equation $i\mathcal{D}_0\Psi|_j = \mathcal{H}'_{Q=0}\Psi_j$ delivers $\mathcal{D}_0^2\Psi|_j = -(\mathcal{H}'_{Q=0})^2\Psi_j$, with $(\mathcal{H}'_{Q=0})^2 = -(A^1)^2\mathcal{D}_1^2 + (\epsilon m)^2(A^0)^2 + \epsilon m[A^0A^1 + A^1A^0](-i\mathcal{D}_1)$. Thanks to the Dirac-continuum-limit constraints, we obtain the correct Klein-Gordon equation in the continuum limit (divide by ϵ^2 and let $\epsilon \to 0$ after a Taylor expansion at second order).

Now, we wish that the discrete scheme obtained by squaring Eq. (4) be a valid discretization of the Klein-Gordon equation, and by "valid" we mean not only that it delivers the correct continuum limit but also that it be applicable, at the discrete level, to scalar state sequences (as is the case in the continuum setting), and for this *we need to impose* $(A^0) \propto 1$ *and* $(A^1)^2 \propto 1$, i.e., *not operator valued* [23], as well as $A^0A^1 + A^1A^0 \propto 1$ or $= 0$. *We choose to impose that the A operators* A^0 *and* A^1 *satisfy* $A^0A^1 + A^1A^0 = 0$, i.e., we impose that the crossed term vanishes (which may be taken as part of the definition of what we consider a valid discrete Klein-Gordon scheme). To sum up, what we impose is that the A operators satisfy the same algebra as that of the α operators of the DE up to multiplicative factors; that is, we impose

$$(A^0)^2 \propto 1, \tag{5a}$$

$$(A^1)^2 \propto 1, \tag{5b}$$

$$A^0A^1 + A^1A^0 = 0. \tag{5c}$$

We now have to find A operators which satisfy (i) this algebra, (ii) the Dirac-continuum-limit constraints, and (iii) the unitarity constraints. Can we find such operators? We are going to see that the answer is "yes," a result which is *a priori* not trivial at all. The trivial choice $A^1 \propto \alpha^1$, more concretely, $B \propto \alpha^1$, is going to allow us to reach our purpose, so we make this choice. What is untrivial is the proportionality constant, as well as the choice of M (which determines A^0). Indeed, a standard choice for the mass term $\epsilon m A^0$ in the literature is $e^{-i\epsilon m\alpha^0}$, but this term together with $A^1 \propto \alpha^1$ means that constraint (5c) is unsatisfied. The term that is going to allow us to reach our purpose is a suggestion from both Feynman's original scheme [24] and Succi's quantum lattice Boltzmann schemes [25,26] (whereas $e^{-i\epsilon m\alpha^0}$ is a suggestion from multiplicative constructions, here our construction is additive): We choose $M = \mu_\epsilon(1 - i\epsilon m\alpha^0)$, where μ_ϵ is a factor that is imposed on us by one of the unitarity constraints (see Appendix A), namely, $M^\dagger M = 1$, so that $\mu_\epsilon := \frac{1}{\sqrt{1+\epsilon^2m^2}}$. This μ_ϵ is also the proportionality factor evoked above: We choose $B := \mu_\epsilon\alpha^1$. The algebra (5a)–(5c) is thus now satisfied, since $A^0 = \mu_\epsilon\alpha^0$ and $A^1 = \mu_\epsilon\alpha^1$, and this algebra is equivalent to the following Clifford algebra: $\{\Gamma^\mu, \Gamma^\nu\} = 2\tilde{\eta}^{\mu\nu}$, where $\{\cdot,\cdot\}$ is the anticommutator and where we have introduced the modified Minkowski metric $\tilde{\eta} := \mathrm{diag}(1/\mu_\epsilon^2, -1)$, as well as the Γ operators $\Gamma^0 := (A^0)^{-1} = \alpha^0/\mu_\epsilon$ and $\Gamma^1 := (A^0)^{-1}A^1 := \alpha^0\alpha^1 := \gamma^1$. One can check that the other and last unitarity constraint involving M but not V, namely, $B^\dagger M = M^\dagger B$, is satisfied.

Let us recap how M is built: The "α^0" in M is both for the unitarity constraint $B^\dagger M = M^\dagger B$ to be satisfied and so that $A^0A^1 + A^1A^0 = 0$; the "ϵm" in front of the α^0 is for the continuum limit to be a good one; the "i" is because $A^0 \propto i(M - M^\dagger)$; and finally, the additional term "1" is for the unitarity constraint $M^\dagger M = 1$ to be satisfied. Now, finally, for the unitarity constraints on V to be satisfied, we can choose $V := \mu_\epsilon$. With these choices for B, M, and V, our DQW with $Q = 0$ is invariant under unitary transformations of the coin state, in such a way that the algebra (5a)–(5c) is preserved, in exact parallel with the continuum situation.

Note that the operators A^0 and A^1 depend on the mass, while in the continuum limit none of the α operators do. Note also that $\mathcal{H}'_{Q=0} = \mu_\epsilon[\alpha^1(-i\mathcal{D}_1) + \epsilon m\alpha^0]$ (and $(\mathcal{H}'_{Q=0})^2 = \mu_\epsilon^2[-\mathcal{D}_1^2 + (\epsilon m)^2]$), with $\mu_\epsilon \neq 1$ if $\epsilon m \neq 0$ (although $\mu_\epsilon \to 1$ as $\epsilon m \to 0$), which is the price one has to pay to obtain a unitary discretization while nevertheless discretizing the transport term naively, by a symmetric finite difference $\mathcal{D}_1$. Finally, let us mention the following: In Appendix A, we have only written the unitarity constraints ensuing from $\mathcal{U}^\dagger\mathcal{U} = 1$, but one can check that the unitarity constraints ensuing from $\mathcal{U}\mathcal{U}^\dagger = 1$ are also satisfied with our choices for B, M, and V.

VII. TOWARDS AVOIDING FERMION DOUBLING WITH THE WILSON Q TERM

Consider the two-step Hamiltonian of Eq. (3) for a nonvanishing Wilson Q term; it is convenient, in order to further take a continuum limit, to rather consider the Hamiltonian $h := \mathcal{H}/\epsilon$ (from the continuum point of view, this is actually the correct Hamiltonian dimensionally). The reason we have referred to the Wilson Q term that way is because its spatial-operator part, $-\mathcal{L}$, is that of the well-known Wilson term of LGT, namely, $(r\epsilon/2)\alpha^0(-\mathcal{L}/\epsilon^2)$ [27], i.e., the same as ours but with α^0 instead of Q. In LGT, this term enables one to avoid the so-called fermion doubling problem, which appears when discretizing the DE naively; these facts are recalled in Appendix B. It is remarkable that such a Wilson term is naturally contained in the decomposition of a generic DQW. What Q can we take in order for fermion doubling to be avoided, while satisfying the unitarity constraints? Is this even possible? We are going to see that the answer to the last question is "yes," a result that is *a priori* not trivial at all.

VIII. KLEIN-GORDON-SQUARE REQUIREMENT WITH THE WILSON Q TERM

Assuming $A^0A^1 + A^1A^0 = 0$, we have that $h^2 = -(A^1)^2\frac{\mathcal{D}_1^2}{\epsilon^2} + m^2(A^0)^2 + \frac{r^2}{4\epsilon^2}Q^2\mathcal{L}^2 + m\frac{r}{2\epsilon^2}[QA^0 + A^0Q](-\mathcal{L}) + \frac{r}{2\epsilon^2}[QA^1 + A^1Q](-\mathcal{L})(-i\mathcal{D}_1)$. Notice that the last three terms vanish in the continuum limit, so that we recover the Klein-Gordon equation. Now, the validity of the discrete Klein-Gordon scheme, which we define, as before, as the possibility of applying the scheme to scalar state sequences, can be obtained if we require, in addition to the previous Clifford-algebra requirement, Eqs. (5a)–(5c), that as $\epsilon \to 0$, (i) $Q^2 \sim 1$ and (ii)

each of the two anticommutators involving Q either vanishes or is proportional to the identity; these requirements suggest that we use for the choice of V the same trick as was used for the choice of M.

Hence we choose the ansatz $V = \nu_\epsilon(1 + i\epsilon^\rho r\alpha^\lambda)$, where (i) α^λ is an α operator satisfying the usual algebra of the α operators of the DE, (ii) ν_ϵ is a normalization factor to be determined, and (iii) ρ is an exponent to be determined. Since we are in one spatial dimension, λ should only take two possible values, $\lambda = 0$ and $\lambda = 1$ (since α^λ has been defined as an α operator of the DE and we are in one spatial dimension). That being said, and we mention this since it is going to be used further down, in general terms: Let us say that we are in n spatial dimensions (so that λ can take values from 0 to n) with a given representation of the Clifford algebra; then λ can take an additional value $n + 1$ provided that in $n + 1$ spatial dimensions one can still find a representation of the Clifford algebra which has the same dimension as the representation found in dimension n [28]. We know that this is precisely the case when going from one spatial dimension to two: For example, if α^0 and α^1 are represented by two Pauli matrices, then we can choose an α^2 that is represented by the last Pauli matrix. Hence we consider that $\lambda = 0$, 1, or 2.

The unitarity constraint $B^\dagger V = V^\dagger B$ requires $\lambda \neq 1$, which we assume, so that the anticommutator $QA^1 + A^1Q$ vanishes. We do not change our choice of M or its normalization factor (the latter enables us to satisfy $M^\dagger M = 1$). Now, both $\lambda = 0$ and $\lambda = 2$ are compatible with the unitarity constraint $2V^\dagger V = V^\dagger M + M^\dagger V$, which determines the following associated normalization factors: $\nu_\epsilon^{\lambda=0} := \mu_\epsilon \frac{1-\epsilon^{1+\rho}mr}{1+(\epsilon^\rho r)^2}$ and $\nu_\epsilon^{\lambda=2} := \frac{\mu_\epsilon}{1+(\epsilon^\rho r)^2}$. Finally, for the unitarity constraint $V^\dagger V = B^\dagger B$ to be satisfied, we need to change the normalization factor for B: We choose $B := \eta_\epsilon^\lambda \alpha^1$, and η_ϵ^λ is determined by the constraint just mentioned, yielding $\eta_\epsilon^\lambda := \nu_\epsilon^\lambda\sqrt{1 + (\epsilon^\rho r)^2}$. All unitarity constraints are now satisfied, including those coming from $\mathcal{U}\mathcal{U}^\dagger = 1$. Now, since μ_ϵ goes to 1 in the continuum limit, we see that for both ν_ϵ^λ and η_ϵ^λ to go to 1 in the continuum limit, we must choose $\rho > 0$: This finally yields $Q = \nu_\epsilon\epsilon^\rho\alpha^\lambda$, which in the continuum limit goes as $\epsilon^\rho\alpha^\lambda$—that is, in the case of $\lambda = 0$, as $\epsilon^\rho\alpha^0$ and not as α^0 as in standard LGT. We finally have

$$h^\lambda = \eta_\epsilon^\lambda\alpha^1\left(\frac{-i\mathcal{D}_1}{\epsilon}\right) + \mu_\epsilon m\alpha^0 + \nu_\epsilon^\lambda\epsilon^\rho\frac{r}{2\epsilon}(-\mathcal{L})\alpha^\lambda. \tag{6}$$

We will keep working with both models $\lambda = 0$ and $\lambda = 2$ and see whether one performs better than the other at avoiding fermion doubling (avoidance which for now is not a given; we are precisely going to explain further down at which condition fermion doubling is avoided).

IX. AVOIDING FERMION DOUBLING

To find solutions of our two-step scheme, Eq. (4), we consider a superposition-of-plane-waves ansatz (since the solution of the DE, which we seek to simulate, has this form): $\Psi(t, x) = \frac{1}{2\pi N}\sum_{i=+,-}\int_{-\infty}^{+\infty} dk\, \tilde{\Psi}_i(0, k)e^{-i(\omega_i(k)t-kx)}$, where $(t, x) = (t_j, x_p)$. Inserting the plane-wave ansatz into Eq. (4) with $h = \mathcal{H}/\epsilon$ given by Eq. (6) leads, after squaring, to a dispersion relation

$$\frac{\sin^2[\omega_i(k)\epsilon]}{\epsilon^2} = F^{\mathrm{DQW},\lambda}(k), \tag{7}$$

where

$$F^{\mathrm{DQW},\lambda=0}(k) := \left(\eta_\epsilon^0\right)^2\frac{\sin^2(k\epsilon)}{\epsilon^2} + \left[\mu_\epsilon m + \nu_\epsilon^0\epsilon^\rho\frac{r}{\epsilon}(1 - \cos(k\epsilon))\right]^2, \tag{8a}$$

$$F^{\mathrm{DQW},\lambda=2}(k) := \left(\eta_\epsilon^2\right)^2\frac{\sin^2(k\epsilon)}{\epsilon^2} + (\mu_\epsilon m)^2 + \left[\nu_\epsilon^2\epsilon^\rho\frac{r}{\epsilon}(1 - \cos(k\epsilon))\right]^2. \tag{8b}$$

Now, discrete-time LGT is usually formulated in a Lagrangian way [29,30], whereas we formulated our discrete-time scheme in a Hamiltonian one. In Lagrangian LGT, a term is naturally added to the action to remove the temporal doublers along with the term added to remove the spatial doublers. Here, this is not the case, and we only treat spatial doublers. Considering a low-frequency limit, $\omega_i(k) \ll 1$, of the dispersion relation finally leads to the solutions

$$\omega_\pm^{\mathrm{DQW},\lambda}(k) = \pm\sqrt{F^{\mathrm{DQW},\lambda}(k)}. \tag{9}$$

Expressions (8a) and (8b) are to be compared with the dispersion relation of standard LGT,

$$F^{\mathrm{LGT}}(k) := \frac{\sin^2(k\epsilon)}{\epsilon^2} + \left[m + \frac{r}{\epsilon}(1 - \cos(k\epsilon))\right]^2. \tag{10}$$

The difference between $F^{\mathrm{DQW},\lambda=0}(k)$ and $F^{\mathrm{DQW},\lambda=2}(k)$ is, apart from the normalization factors ν_ϵ^λ and η_ϵ^λ, the *crossed term* of the square of the sum in $F^{\mathrm{DQW},\lambda=0}(k)$. In standard LGT, this crossed term is also present. Since the upcoming discussion is the same whether there is a crossed term or not, let us forget about the latter for now; we will come back to it later. Here comes the discussion. In standard LGT, what allows fermion doubling to be avoided is that the function $1 - \cos(k\epsilon)$ raises the value of the dispersion relation at the edges of the Brillouin zone, i.e., at $\pm\pi/\epsilon$. More precisely, if the amplitude by which this dispersion relation is raised, which we call the *raising amplitude*, does not go to zero with ϵ, then for sure fermion doubling is avoided, and this is indeed the case in standard LGT since the associated raising amplitude is $(r/\epsilon)^2$; see Eq. (10). In our model, the raising amplitude is $(\nu_\epsilon^\lambda r\epsilon^{\rho-1})^2$; see Eqs. (8a) and (8b). Since ν_ϵ^λ goes to 1 in the continuum limit, we are fine as long as

$$\rho < 1; \tag{11}$$

that is, this condition ensures that fermion doubling is avoided, both for $\lambda = 0$ and $\lambda = 2$.

X. INITIAL SLOPES

The limit to the continuum is obtained by letting ϵ go to zero. Let us consider the gapless frequencies

$$f^{\mathrm{M}}(k) := \sqrt{[\omega_\pm^{\mathrm{M}}(k)]^2 - M^{\mathrm{M}}} = \sqrt{F^{\mathrm{M}}(k) - M^{\mathrm{M}}}, \tag{12}$$

where "M" is the considered model and takes for now the "values" M = (DQW, $\lambda = 0$) or M = (DQW, $\lambda = 2$) and where M^{M} is the central ($k = 0$) gap of the model. Let us consider the Taylor expansion of the dispersion relations $(f^{\mathrm{M}}(k))^2$ at next-to-lowest order in ϵ. *A priori*, the two Taylor-expanded dispersion relations (one for $\lambda = 0$ and one for $\lambda = 2$) are different: More precisely, there are *a priori* more terms in the case of $\lambda = 0$, namely, the crossed terms. Now, it turns out that these additional terms actually cancel each other, at least at next-to-lowest order in ϵ, so that both the model $\lambda = 0$ and the model $\lambda = 2$ have, at next-to-lowest order in ϵ, the same Taylor expansion in ϵ, namely,

$$(f^{\mathrm{DQW},\lambda=0}(k))^2 \simeq (f^{\mathrm{DQW},\lambda=2}(k))^2 \simeq \left(1 - \frac{1}{2}r^2\epsilon^{2\rho}\right)k^2. \quad (13)$$

Actually, even if these above-mentioned additional terms had not canceled each other, they would be of higher order because $\rho < 1$, so both model $\lambda = 0$ and model $\lambda = 2$ would still have the same small-ϵ expansion; we leave the verification of this observation to the reader. Moreover, the criterion $\rho < 1$ for the avoidance of fermion doubling in our model is the same whether there is a crossed term or not. Hence we consider both model $\lambda = 0$ and model $\lambda = 2$ equivalently good for our task of avoiding fermion doubling and converging as fast as possible to the continuum limit. We choose $\lambda = 0$, in order for comparisons to LGT to be simpler, and from now on we call this model M = DQW. At this point the reader may wonder why we have kept the discussion about $\lambda = 0$ and $\lambda = 2$ if in the end we consider both models equivalently good and choose, e.g., $\lambda = 0$: Apart from a mere informative reason, this discussion is going to be useful just below in the next paragraph, to understand the role of the crossed term in the LGT model at small ϵ, and the subsequent interest of getting rid of this crossed term by choosing $\lambda = 2$ in this LGT model.

We call the factor in front of k^2 in Eq. (13) the (squared) initial slope of the model. In standard LGT, the lowest-order modification of the initial slope comes, this time, from the crossed term (this is detailed in Appendix B): At next-to-lowest order in ϵ we have that

$$(f^{\mathrm{LGT}}(k))^2 \simeq (1 + \epsilon mr)k^2. \quad (14)$$

Hence, for the initial slope of our model to converge faster to the continuum limit than that of the LGT model, we need to choose

$$\rho > 0.5. \quad (15)$$

In the end, we have, in addition to in-built unitarity, a model that performs better at reaching the continuum limit than that of LGT if we choose $\rho \in]0.5, 1[$. That being said, if we choose in the LGT model $\lambda = 2$, then the initial slope is exactly that of the continuum, that is, 1 (we leave the verification of this to the reader), and in that case the LGT model performs better than ours at reaching the continuum limit, whatever value we choose for ρ.

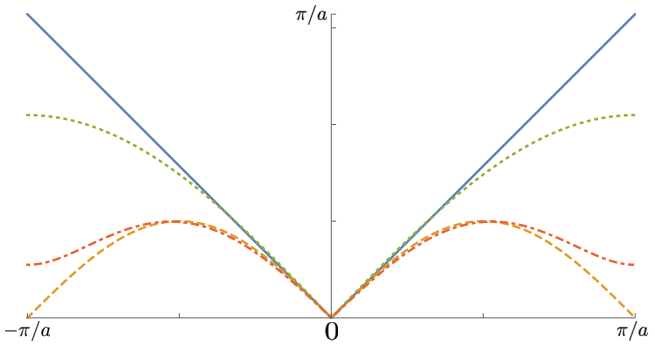

FIG. 1. Gapless frequency $f^{\mathrm{M}}(k)$ of model "M", for "M" = "Dirac" (blue, solid curve), "naive" (gold, dashed curve), "LGT" (green, dotted curve), and "DQW" (red, dot-dashed curve), where $f^{\mathrm{Dirac}}(k) = |k|$, $f^{\mathrm{naive}}(k) = \frac{|\sin(k\epsilon)|}{\epsilon}$, $f^{\mathrm{LGT}}(k) = \sqrt{\frac{\sin^2(k\epsilon)}{\epsilon^2} + \left[m + \frac{r}{\epsilon}(1 - \cos(k\epsilon))\right]^2 - m^2}$, and $f^{\mathrm{DQW}}(k) = \sqrt{(\eta_\epsilon^0)^2\frac{\sin^2(k\epsilon)}{\epsilon^2} + \left[\mu_\epsilon m + \nu_\epsilon^0\epsilon^\rho\frac{r}{\epsilon}(1 - \cos(k\epsilon))\right]^2 - (\mu_\epsilon m)^2}$, for $\epsilon = 0.1$, $m = 1$, $r = 1$ (Wilson's choice), and $\rho = 0.6$.

XI. GAPLESS FREQUENCIES OF THE DIFFERENT MODELS

In Fig. 1, we plot the gapless frequencies defined above in Eq. (12), where this time the model M takes the "values" M = Dirac, naive, LGT, DQW. We see that the naive discretization of the DE leads to two extra poles in the gapless frequency (gold curve), which causes the fermion doubling problem (see Appendix B), while the LGT (green curve) and DQW (red curve) models avoid it by creating gaps at the edges. In-built unitarity *for any* $r \in \mathbb{R}$ is an important advantage of our model with respect to LGT.

Take a closer look at the initial slopes (i.e., around $k = 0$). One can appreciate, though weakly, the fact that the initial slope of the DQW (LGT) model is a bit smaller (bigger)—see Eq. (13) [Eq. (14)]—than that of Dirac fermions (although the two former slopes obviously converge to the latter in the continuum limit, i.e., for ϵ going to 0). We could have made this fact more visible in Fig. 1; however, if we had done so, the curves would not have given the impression (which is anyway of course a truth, as shown above) that in the continuum limit one does get the correct initial slope, while in Fig. 1 as presented this impression is given.

Let us make a final remark. In Fig. 1, we have chosen $r = 1$ because it is a standard choice. That being said, let us mention that for $r = 1$ the discrete-time LGT model of Wilson fermions (which is a Lagrangian model) can actually be proven to be unitary. This proof does, however, not hold for $r \neq 1$ [30], while our model has in-built unitarity for any r. Pay attention that if we choose, for $r = 1$, $\lambda = 2$ in the discrete-time LGT model, unitarity would again have to be proven, and it may actually not hold.

XII. CONCLUSION

We showed that a Clifford algebra emerges out of the internal-state operators defining a quantum-automaton discretization of the Dirac equation. This discretization, which

is a DQW, is unitary by construction, while discrete-time versions of lattice gauge theory are usually Lagrangian so that unitarity is not in-built. Our DQW is invariant under representation changes of the above-mentioned Clifford algebra, which parallels exactly the continuum situation. Moreover, we show that DQWs naturally contain a Wilson term that allows spatial fermion doubling to be avoided, and this is the case without breaking unitarity and for any choice $r \in \mathbb{R}$ of Wilson's parameter.

The $(3+1)$D extension of the present work should be investigated. Let us give some guidelines on this matter. The reader can check that the present DQW, Eq. (1)—with the operators finally chosen for W_{-1}, W_0, and W_1—can almost be seen as a generalization, for an arbitrary representation of the Clifford algebra, of the automaton presented in Refs. [6,31]. Hence one could look for $(3+1)$D generalizations of the automaton presented in Ref. [6]: Such a generalization is presented in Refs. [32,33]. One question would then be, Can we go from the $(3+1)$D DQW of Refs. [32,33] to a generalization for an arbitrary Clifford algebra, exactly as we go from the $(1+1)$D DQW of Ref. [6] to the generalization presented in this paper? The idea just suggested here is to look for $(3+1)$D schemes which are *additive* [32,33], rather than *multiplicative* [8,34]. That being said, maybe combining $(1+1)$D additive schemes (one such scheme for each spatial dimension) in a multiplicative way can (also?) do the job.

Regarding the coupling to gauge fields, the author of this paper is carrying out work on this matter, based on Ref. [35]: It appears that a natural gauging (i.e., via the procedure described in Ref. [35]) of the one-step scheme, Eq. (1), is not fully equivalent to a natural gauging (i.e., via the procedure standardly followed in LGT, which actually seems to be the same as that of Ref. [35]) of the two-step scheme, so some care is in order regarding this matter. In other words, gauging a one-step scheme is not fully equivalent to gauging a two-step scheme.

ACKNOWLEDGMENTS

The author thanks C. Cedzich for making him notice that the two-step Hamiltonian is (ultra)local, while the effective Hamiltonian, as a logarithm of the one-step evolution operator, is not (infinite series of growing powers of the one-step evolution operator). This is an interesting feature which is in the prolongation of the ultralocality of the one-step evolution operator that is sought in the development of quantum cellular automata and their one-particle versions, DQWs. The author also thanks A. Grinbaum for energetic stylistic and grammatical advice and corrections.

APPENDIX A: UNITARITY CONSTRAINTS

In this Appendix, we translate, on the transport coin operators B, V, and M, the unitarity constraints imposed on the jump coin operators W_i, $i=-1,0,1$, by the unitarity of the one-step evolution operator $\mathcal{U}$.

We impose the unitarity of $\mathcal{U}$, that is, $\mathcal{U}^\dagger\mathcal{U}=1$. A couple of computation lines lead to the following conditions on the jump coin operators W_i, $i=-1,0,1$, which we call unitarity constraints on the jump coin operators:

$$W_{-1}^\dagger W_{-1} + W_1^\dagger W_1 + W_0^\dagger W_0 = 1, \tag{A1a}$$

$$W_{-1}^\dagger W_0 + W_0^\dagger W_1 = 0, \tag{A1b}$$

$$W_{-1}^\dagger W_1 = 0. \tag{A1c}$$

Let us translate these constraints on the transport coin operators B, V, and M. We start with constraint (A1c), which is the simplest to translate in the sense that it does not involve M while both constraints (A1a) and (A1b) do. Constraint (A1c) yields

$$0 = (V^\dagger - B^\dagger)(V+B) \tag{A2a}$$

$$= V^\dagger V - B^\dagger B - B^\dagger V + V^\dagger B. \tag{A2b}$$

Computing the sum and the difference, $(A2b)^\dagger+$ and $(A2b)^\dagger-$(A2b), yields

$$\boxed{V^\dagger V = B^\dagger B,} \tag{A3a}$$

$$\boxed{B^\dagger V = V^\dagger B,} \tag{A3b}$$

respectively. Conversely, it is trivial to check that these two constraints imply constraint (A1c).

We now proceed with translating constraint (A1b), because we will use one of the two resulting constraints to translate constraint (A1a). Constraint (A1b) yields

$$0 = (V^\dagger - B^\dagger)(M-V) + (M^\dagger - V^\dagger)(V+B) \tag{A4a}$$

$$= V^\dagger M - B^\dagger M - V^\dagger V + B^\dagger V + M^\dagger V - V^\dagger V + M^\dagger B - V^\dagger B. \tag{A4b}$$

Computing the sum and the difference, $(A4b)^\dagger+$(A4b) and $(A4b)^\dagger-$(A4b), and using Eq. (A3b) in the difference, yields

$$\boxed{2V^\dagger V = V^\dagger M + M^\dagger V,} \tag{A5a}$$

$$\boxed{B^\dagger M = M^\dagger B,} \tag{A5b}$$

respectively. Conversely, it is trivial to check that these two constraints together with constraint (A3b) imply constraint (A1b).

We finally proceed with translating constraint (A1a), which can be written

$$4 = (V^\dagger - B^\dagger)(V-B) + (V^\dagger + B^\dagger)(V+B) + 4W_0^\dagger W_0 \tag{A6a}$$

$$= V^\dagger V + B^\dagger B - B^\dagger V - V^\dagger B + V^\dagger V + B^\dagger B + B^\dagger V + V^\dagger B + 4W_0^\dagger W_0. \tag{A6b}$$

Inserting both constraint (A3a) and constraint (A3b) into the preceding one, constraint (A6b), delivers

$$1 = V^\dagger V + W_0^\dagger W_0 \tag{A7a}$$

$$= V^\dagger V + (M^\dagger - V^\dagger)(M-V) \tag{A7b}$$

$$= 2V^\dagger V + M^\dagger M - M^\dagger V - V^\dagger M. \tag{A7c}$$

Finally, inserting constraint (A5a) into the preceding one, constraint (A7c), results in

$$\boxed{M^\dagger M = 1.} \tag{A8}$$

APPENDIX B: FERMION DOUBLING AND WILSON FERMIONS IN CONTINUOUS AND DISCRETE TIME

In this Appendix, we explain the fermion doubling problem of lattice gauge theory and present Wilson's method to solve it, with so-called Wilson fermions.

1. The Schrödinger equation for translationally invariant systems

a. The generic Schrödinger equation and its spectral solution

The generic Schrödinger equation is a partial differential equation (PDE) of the form

$$i\partial_0 \Psi|_t = h\Psi(t), \tag{B1}$$

where h is a Hermitian linear operator acting on the function $\Psi(t) : x \mapsto \Psi(t,x)$, where here we choose $x \in \mathbb{R}$. Since this equation is linear, we solve it spectrally, i.e., by finding the eigenelements $(\omega_\sigma, \Phi_\sigma)_{\sigma\in\Sigma}$ of h, where Σ is a certain indexing space; by definition, these eigenelements satisfy

$$h\Phi_\sigma = \omega_\sigma \Phi_\sigma, \tag{B2}$$

where the eigenvalues ω_σ are real since h is Hermitian.

The method is the following. Assume we have determined the eigenelements of h. Since $\Psi(t)$ belongs to a Hilbert space, we can decompose it on the eigenbasis $(\Phi_\sigma)_{\sigma\in\Sigma}$ at an arbitrary time t:

$$\Psi(t) = \sum_{\sigma\in\Sigma} C_\sigma(t)\Phi_\sigma, \tag{B3}$$

where the $C_\sigma(t)$'s are the coefficients of $\Psi(t)$ on the eigenbasis. Now, using Eq. (B2), the generic Schrödinger equation on Ψ, Eq. (B1), which is a PDE, can be translated into a family of ordinary differential equations (ODEs)–indexed by σ—for the coefficients C_σ, that is,

$$i\partial_0 C_\sigma|_t = \omega_\sigma C_\sigma(t), \tag{B4}$$

whose solution is well known:

$$C_\sigma(t) = C_\sigma(0)e^{-i\omega_\sigma t}. \tag{B5}$$

Hence the solution sought is

$$\boxed{\Psi(t) = \sum_{\sigma\in\Sigma} C_\sigma(0)e^{-i\omega_\sigma t}\Phi_\sigma.} \tag{B6}$$

Because they intervene in the periodic functions $t \mapsto e^{-i\omega_\sigma t}$, the ω_σ are called *frequencies*; more precisely, they are the *eigenfrequencies of* h. To be more definite, one should actually use the denomination "angular frequency" rather than "frequency."

b. Fourier analysis

We will use the more definite notation $\Psi(t,\cdot)$ for $\Psi(t)$ when needed. Let us take the Fourier transform of $\Psi(t,\cdot)$ at a given time t:

$$\tilde\Psi(t,k) := \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} dx\, \Psi(t,x)e^{-ikx}. \tag{B7}$$

Inverting this equation, we obtain the decomposition of $\Psi(t)$ into its Fourier components:

$$\Psi(t,x) = \frac{1}{\sqrt{2\pi}}\int_{\mathbb{R}} dk\, \tilde\Psi(t,k)e^{ikx}. \tag{B8}$$

To be precise, the function $x \mapsto \tilde\Psi(t,k)e^{ikx}$ is the *Fourier component* of $\Psi(t,\cdot)$ associated with the value k of the Fourier variable, and $\tilde\Psi(t,k)$ is the *Fourier coefficient*, or *Fourier amplitude* of $\Psi(t,\cdot)$ associated with the value k. Because x is a spatial position, the Fourier variable k is a *spatial frequency*; again, as in the case of ω_σ above, to be more definite, one should use the denomination "angular pulsation" rather than "frequency."

c. Case of translationally invariant systems

If h does not depend on the point x, i.e., if h is translationally invariant, then one can check by considering Eq. (B1) for expression (B8) that each Fourier coefficient satisfies the equation

$$i\partial_0\tilde\Psi(\cdot,k)|_t = \tilde h(k)\tilde\Psi(t,k), \tag{B9}$$

where $\tilde h(k)$ is the expression obtained when replacing, in h, the operator $-i\partial_1$ by the real number k.

Hence, if h does not depend on the point x, each Fourier coefficient evolves independently of the others, while this is not the case if h does depend on x. Moreover, the "Schrödinger equation in Fourier space," Eq. (B9), is simpler to solve than the original Schrödinger equation, (B1), because the operator $-i\partial_1$ has been replaced by a real number k, so that Eq. (B9) is not a PDE, like the original Schrödinger equation, but a *family* of ODEs indexed by k. Let us now make the link with Appendix B 1a: One can actually mathematically show (via, e.g., "mere" constructive proofs) for a large class of operators h, that there exists an indexing space Σ such that k is one of the indices, i.e., $k \in \sigma$ [36]. In the language of quantum mechanics, an index $i \in \sigma$ is referred to as a good quantum number; it is an eigenvalue of an operator whose diagonalization serves as a partial diagonalization of h, i.e., h is codiagonalizable with that operator.

We often speak of *Fourier modes* for the Fourier components: The term "mode" refers, in its most general acceptation, to one of the terms of a particularly relevant decomposition of an object; take, e.g., the Fourier decomposition of a function. In the case of an x-independent h, the Fourier modes are actually *proper modes*, because by considering the Fourier version $\tilde h(k)$ of h we have (at least partially) "diagonalized" h (which is summed up by writing $k \in \sigma$).

2. The solution of the Schrödinger equation for translationally invariant systems: A superposition of plane waves

a. No internal structure for $\Psi(t,x)$

i. Final solution. If $\Psi(t,x)$ has no internal structure, i.e., if $\Psi(t,x) \in \mathbb{C}$, then we simply have that $k = \sigma$, and the eigenvalues are $\omega_\sigma = \omega(k) := \tilde h(k) \in \mathbb{R}$; the sum over σ in Eq. (B6) is an integral over k, and the eigenbasis is the following family of functions of x: $(\Phi(\cdot,k))_{k\in\mathbb{R}}$, with

$$\Phi(x,k) := \frac{e^{ikx}}{\sqrt{2\pi}}. \tag{B10}$$

Therefore the solution given in Eq. (B6) here reads

$$\Psi(t,x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dk\, C(0,k)\, e^{-i(\omega(k)t - kx)}. \tag{B11}$$

By taking $t = 0$ in this equation we realize by identification (they are unique) that the $C(0,k)$ are the Fourier coefficients of $x \mapsto \Psi(0,x)$, i.e.,

$$C(0,k) \equiv \tilde{\Psi}(0,k). \tag{B12}$$

The value $\omega(k)$ is the eigenfrequency associated with the spatial frequency k. Now, an important remark is that $\Psi(t,\cdot)$ is actually a superposition of plane waves, with weights being the Fourier coefficients of the initial condition. Because of this (plane-)wave structure, the spatial frequency k is called a *wave vector* [37]. The fact that the frequency of the wave $\omega(k)$ depends on the wave vector k is called *dispersion*, and the expression $\omega(k)$ is called the *dispersion relation*. Notice that the fact that we have a dispersion phenomenon while we are in a vacuum is specific to quantum mechanics, more precisely, to the quantum mechanics of massive bodies.

In quantum mechanics, the use of the word "wave vector" is actually extended to non-translationally-invariant systems, because this wave vector is, due to the wave-particle duality, in one-to-one correspondence with the momentum of the free particle associated with the wave in question, the solution of a free (i.e., with x-independent h) Schrödinger equation: More precisely, k is the de Broglie wave vector of a particle of momentum $p = k$ (with $\hbar = 1$). There is also an analog relation for the eigenfrequencies, referred to as Einstein's relation: The frequency ω_σ is the frequency associated with an energy $E_\sigma = \omega_\sigma$ (with $\hbar = 1$) for the particle in question.

ii. Final solution rederived by focusing on the linear algebraic structure. One has the opportunity to rederive the above solution, Eq. (B11), by focusing on the linear algebraic structure of the computations. This will make gentler the above replacement of σ by k. We first rewrite Eq. (B6) with a bra-ket notation, which emphasizes the linear algebraic structure,

$$|\Psi(t)\rangle = \sum_{\sigma\in\Sigma} \underbrace{\langle \Phi_\sigma | \Psi(0)\rangle}_{\equiv C_\sigma(0)} e^{-i\omega_\sigma t} |\Phi_\sigma\rangle . \tag{B13}$$

By taking $t = 0$ in this equation, we see that we have simply applied the closure relation $\sum_{\sigma\in\Sigma} |\Phi_\sigma\rangle\langle\Phi_\sigma|$ to $|\Psi(0)\rangle$ and then evolved the eigenstates up to time t. We then consider the present case $\sigma = k$, so that $\Phi_\sigma = \Phi(\cdot,k)$, which means that the eigenbasis is the basis made up of the $|k\rangle := |\Phi(\cdot,k)\rangle$ with $k \in \mathbb{R}$,

$$|\Psi(t)\rangle = \int_{\mathbb{R}} dk\, \underbrace{\langle k | \Psi(0)\rangle}_{\equiv \tilde{\Psi}(0,k)} e^{-i\omega_\sigma t} |k\rangle . \tag{B14}$$

We then apply the bra $\langle x|$ to have the value at point x,

$$\langle x|\Psi(t)\rangle = \int_{\mathbb{R}} dk\, \tilde{\Psi}(0,k) e^{-i\omega_\sigma t} \langle x|\Phi(\cdot,k)\rangle, \tag{B15}$$

which is, using Eq. (B10), exactly Eq. (B11),

$$\boxed{\Psi(t,x) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} dk\, \tilde{\Psi}(0,k) e^{-i(\omega(k)t - kx)}.} \tag{B16}$$

b. Internal structure for $\Psi(t,x)$

Now, if $\Psi(t,x)$ has an internal structure, then $k \subsetneq \sigma$ [38], and $\tilde{h}(k)$ can be seen as a matrix indexed by k, which one has to diagonalize to finally find the eigenvalues of h. The eigenvalues of $\tilde{h}(k)$ can be denoted $\omega_\sigma = \omega_i(k)$, where $i = 1,\ldots,d$, with d being the dimension of the matrix $\tilde{h}(k)$ [some eigenvalues may be equal, e.g., $\omega_{i_a}(k) = \omega_{i_b}(k)$]. The final solution is then

$$\boxed{\Psi(t,x) = \sum_{i=1}^{d} \frac{1}{\sqrt{2\pi}N} \int_{\mathbb{R}} dk\, \tilde{\Psi}_i(0,k) e^{-i(\omega_i(k)t - kx)},} \tag{B17}$$

where N is a normalization factor, needed if we want the eigenvectors $\tilde{\Psi}_i(0,\cdot)$ of $\tilde{h}(k)$ to be normalized. We see that the solution is still a superposition of plane waves, and there are d dispersion relations $\omega_i(k)$, $i = 1,\ldots,d$.

3. Dirac fermions (continuous spacetime)

The Dirac Hamiltonian in $1+1$ dimensions is

$$\hat{h}^{\text{Dirac}} := \alpha^1 \hat{k} + m\alpha^0, \tag{B18}$$

where $\hat{k}$ is the momentum operator, i.e., the abstract version of the operator $-i\partial_1$, and the alpha matrices satisfy $(\alpha^0)^2 = (\alpha^1)^2 = 1$ and $\alpha^0\alpha^1 + \alpha^1\alpha^0 = 0$. We see that $\hat{h}^{\text{Dirac}}$ is Hermitian, and so it is a valid Hamiltonian for the generic Schrödinger equation considered in Appendixes B 1 and B 2 above. Moreover, it is translationally invariant.

We consider the "Hamiltonian in momentum space,"

$$\tilde{h}^{\text{Dirac}}(k) := \alpha^1 k + m\alpha^0. \tag{B19}$$

The eigenvalue equation with unknowns being the eigenelements $(\omega_i(k), V_i(k))_{i=1,\ldots,d;k\in\mathbb{R}}$ of $\tilde{h}^{\text{Dirac}}(k)$ is, in matrix notation,

$$\tilde{h}^{\text{Dirac}}(k) V_i(k) = \omega_i(k) V_i(k). \tag{B20}$$

Now, to find the eigenvalues of $\tilde{h}^{\text{Dirac}}(k)$, there is actually a "trick," related to the fact that the square of the Dirac equation is, by (historical) construction of the Dirac equation, the Klein-Gordon equation and hence applicable to scalar state functions: The square $(\tilde{h}^{\text{Dirac}}(k))^2$ is proportional to the identity matrix. By squaring Eq. (B20), we arrive at

$$\omega(k)^2 = k^2 + m^2, \tag{B21}$$

so that the eigenvalues are

$$\boxed{\omega_\pm^{\text{Dirac}}(k) := \pm\sqrt{k^2 + m^2}.} \tag{B22}$$

4. The doubling problem when discretizing space but keeping time continuous: Spatial doublers

To discretize space, we can simply perform the naive replacement of the partial derivative ∂_1 by a finite difference on a 1D lattice that we introduce, with sites labeled by $p \in \mathbb{Z}$ and lattice spacing a. The finite difference has to be symmetric if we want the resulting Hamiltonian to be Hermitian. Since the translation operator in the direction of growing p's is, in abstract space, $\hat{T} = e^{-i\hat{k}a}$ [39], the substitution of $\partial_1 = i\mathcal{K}$,

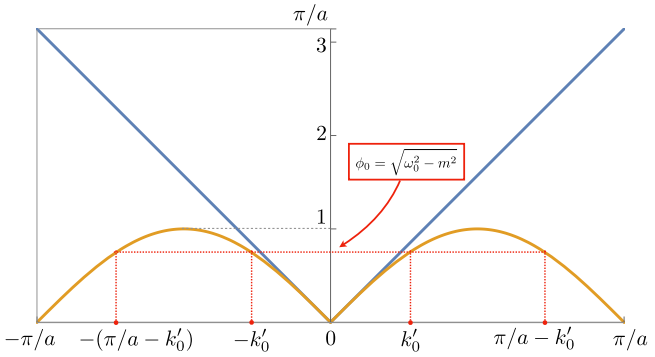

FIG. 2. Illustration of the fermion doubling problem in discrete space but continuous time. The lattice dispersion relation under the form $f_{\text{naive}}(k)$ (in gold) has three poles, $-\pi/a$, 0, and π/a, whereas there is a single one, 0, for the continuum dispersion relation (in blue), so that for each target value ϕ_0 of the gapless frequency, we have two extra momentum solutions on the lattice with respect to the continuum situation.

where $\mathcal{K} := -i\partial_x$, by the announced symmetric finite difference,

$$\mathcal{D}_1 := \tfrac{1}{2}(\mathcal{T}_1^{-1} - \mathcal{T}_1), \tag{B23}$$

corresponds to the following substitution in the "Dirac Hamiltonian in momentum space" $\tilde{h}^{\text{Dirac}}$, as well as in the dispersion relation, Eq. (B22):

$$k \to (-i)\frac{e^{ika} - e^{-ika}}{2a} = \frac{\sin(ka)}{a}. \tag{B24}$$

To explain the doubling problem, it is customary to consider the following function of k:

$$\boxed{f^{\text{naive}}(k) := \sqrt{[\omega_{\pm}^{\text{naive}}(k)]^2 - m^2} \equiv \left|\frac{\sin(ka)}{a}\right|}, \tag{B25}$$

to be compared with

$$f^{\text{Dirac}}(k) := \sqrt{[\omega_{\pm}^{\text{Dirac}}(k)]^2 - m^2} \equiv |k|. \tag{B26}$$

Notice first that the spatial discretization implies that now $k \in [-\pi/a, \pi/a)$. Second, notice that we of course recover the continuum situation for $ka \ll 1$, because $\sin(ka) = ka + O((ka)^3)$. We call the function $f^{\text{M}}(k)$ the gapless frequency of model M.

In Fig. 2, we plot both $f^{\text{Dirac}}(k)$ and $f^{\text{naive}}(k)$ over the Brillouin zone $[-\pi/a, \pi/a)$. The doubling problem is the following. For a given target value $\phi_0 := \sqrt{\omega_0^2 + m^2}$ of the gapless frequency, there are, in the naive discretization, not two possibilities for the momentum as in the continuum situation, k_0 and $-k_0$ such that $f^{\text{Dirac}}(k_0) = \omega_0$, i.e., $k_0 = \omega_0$, but four solutions, two corresponding to the low-momentum modes that we seek to simulate with the discretization, which have $k_0' \simeq k_0$ and $-k_0'$ such that $f^{\text{naive}}(k_0') = \phi_0$, and two additional, high-momentum modes, namely, $\pi/a - k_0'$ and $-(\pi/a - k_0')$, so that frequencies and momenta are not in one-to-one correspondence anymore. In a noninteracting model, i.e., if h does not depend on x, this is actually not a problem because the Fourier modes are independent of each other, and so the one-to-one correspondence between frequency and momentum can be tracked, e.g., fundamentally, as time evolves. More precisely and concretely, in a noninteracting model, the momentum distribution is unchanged by the dynamics; that is, in other words, the states of fixed momentum are stationary states. In an interacting model, the Fourier modes will not evolve independently of each other, and the interaction term will cause the production of high-momentum modes from low-momentum ones—because of the two extra poles of $f^{\text{naive}}(k)$ with respect to $f^{\text{Dirac}}(k)$—which can be proved rigorously in, e.g., perturbative studies of interacting models having as zeroth order $f^{\text{naive}}(k)$ [29,40].

As a conclusion, in discrete space (but keeping time continuous), we will have extra, spurious modes when looking for superpositions of plane waves as Eq. (B17) for the solutions. These spurious modes are called *spatial doublers*, where the specification "spatial" is due to the fact that what is spurious in these modes is the spatial part (high momenta, not compatible with a continuum description, even if the temporal part is—i.e., low frequencies).

5. The doubling problem in discrete spacetime: Temporal doublers in addition to the spatial doublers

We start from the discrete-space-but-continuous-time situation described just above in Appendix B 4, that is,

$$i\partial_0 \Psi(\cdot, x)|_t = h^{\text{naive}} \Psi(t, \cdot)|_x. \tag{B27}$$

As we did for space in Appendix B 4, we discretize time naively, with a symmetric finite difference, in order to treat time on the same footing as space (for which we have indeed used a symmetric finite difference), which yields (replacing h^{naive} by its expression)

$$\frac{i}{2\epsilon}(\Psi(t+\epsilon) - \Psi(t-\epsilon)) = \left[\frac{-i}{2a}(e^{i\mathcal{K}a} - e^{-i\mathcal{K}a})\alpha^1 + m\alpha^0\right]\Psi(t, \cdot)|_x. \tag{B28}$$

Notice right away that this scheme takes two initial conditions, exactly like the two-step scheme we present in this paper; the only difference compared with the two-step scheme we present is that in the latter there is a factor $\mu(\epsilon)$ in front of $m\alpha^0$, but this is enough to make that scheme unitary, while the present, naive one, is not [41]. We consider an ansatz which is a superposition of plane waves with internal components; that is, we look for solutions of the form of Eq. (B17). If we insert Eq. (B17) into Eq. (B28), we obtain after a few computation lines the following equation in momentum space:

$$\frac{\sin[\omega_i(k)\epsilon]}{\epsilon}\tilde{\Psi}_i(0, k) = \left[\frac{\sin(ka)}{a}\alpha^1 + m\alpha^0\right]\tilde{\Psi}_i(0, k). \tag{B29}$$

This equation, squared, and choosing the ballistic scaling $\epsilon = a$, finally yields the following dispersion relation:

$$\sin^2[\omega_i(k)\epsilon] = \sin^2(k\epsilon) + \epsilon^2 m^2. \tag{B30}$$

First of all, notice that for low frequencies $\omega_i(k)\epsilon \ll 1$ in Eq. (B30), we recover the discrete-space-but-continuous-time situation, with gapless frequency given by Eq. (B25) in

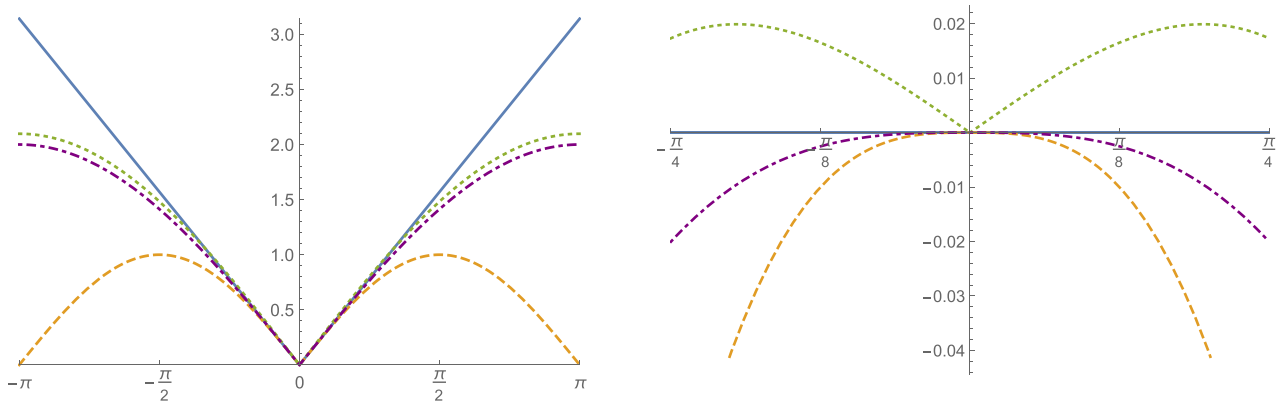

FIG. 3. Gapless frequency $f^{\mathrm{M}}(k)$ of model "M" (left panel) and absolute difference $f^{\mathrm{M}}(k) - f^{\mathrm{Dirac}}(k)$ (right panel), for "M" = "Dirac" (blue, solid curve), "naive" (gold, dashed curve), "LGT" (green, dotted curve), and "LGT noncrossed" (purple, dot-dashed curve), where $f^{\mathrm{Dirac}}(k) = |k|$, $f^{\mathrm{naive}}(k) = \frac{|\sin(ka)|}{a}$, $f^{\mathrm{LGT}}(k) = \sqrt{\frac{\sin^2(ka)}{a^2} + \left[m + \frac{r}{a}(1-\cos(ka))\right]^2 - m^2}$, and $f^{\mathrm{LGT\ noncrossed}}(k) = \sqrt{\frac{\sin^2(ka)}{a^2} + \frac{r^2}{a^2}(1-\cos(ka))^2}$, for $a = 1$, $m = 0.1$, and $r = 1$ (Wilson's choice).

Appendix B 4. Now, there are solutions $\omega_i(k)$ to Eq. (B30) if and only if $|\sin^2(k\epsilon) + \epsilon^2 m^2| \leqslant 1$, which leads to

$$\epsilon^2 m^2 \leqslant \cos^2(k\epsilon). \tag{B31}$$

Replacing in the dispersion relation, Eq. (B30), $\sin^2(A)$ by $(1-\cos(2A))/2$, we obtain the two following solutions:

$$\omega_{\pm}^{\mathrm{temporal}}(k) := \pm\frac{2}{\epsilon}\arccos[1 - 2\sin^2(k\epsilon) - 2\epsilon^2 m^2]. \tag{B32}$$

For small enough k and m, i.e., $k\epsilon \ll 1$ and $\epsilon m \ll 1$, we have that $|\omega_{\pm}^{\mathrm{temporal}}(k)\epsilon| < \pi/2$, and actually that $|\omega_{\pm}^{\mathrm{temporal}}(k)\epsilon| \ll 1$, and these two solutions approach the low frequencies $\omega_{\pm}^{\mathrm{Dirac}}(k)$ of the continuum model.

Now, in addition to these two solutions, Eq. (B32), we also have the solutions

$$\Omega_{\pm}^{\mathrm{temporal}}(k) := \pm\left[\frac{\pi}{\epsilon} - \omega_{\pm}^{\mathrm{temporal}}(k)\right], \tag{B33}$$

which are high-frequency solutions when $|\omega_{\pm}^{\mathrm{temporal}}(k)\epsilon| < \pi/2$. These two extra solutions are spurious because they are not compatible with a continuum description, but they will intervene in the dynamics in interacting models, and the modes associated with these solutions are called *temporal doublers*. As we have seen, these temporal doublers arise even for low momenta [42] (the only ones compatible with a continuum description), and this is best seen as follows. Consider low momenta in Eq. (B30); this yields, replacing k by the notation $\kappa(w)$ and replacing $\omega_i(k)$ by the variable w,

$$g^{\mathrm{naive}}(w) := \sqrt{\kappa(w)^2 + m^2} = \left|\frac{\sin^2(w\epsilon)}{\epsilon}\right|, \tag{B34}$$

an expression which, apart from the fact that there is a $+m^2$ instead of a $-m^2$, corresponds exactly to the expression of the gapless frequency, Eq. (B25), but having exchanged in it the roles of $\omega(k)$ and k, i.e., replaced the latter by $\kappa(w)$ and w, respectively, so that one can derive the same explanations for the temporal doublers as for the spatial doublers. Notice that, in this low-momentum context, the condition (B31) for a solution $\omega_i(k)$ to exist is

$$\epsilon^2 m^2 \leqslant 1 - \tfrac{1}{2}(k\epsilon)^2. \tag{B35}$$

6. Removing the doublers with Wilson fermions

a. We limit ourselves to spatial doublers

In Appendix B 5, we have illustrated the problem of temporal doublers starting from a continuous-time description. A framework which is more appropriate to further remove temporal doublers is that of Lagrangian LGT, which starts from a Lagrangian continuum description rather than a Hamiltonian one. This leads to a modification of the action rather than the Hamiltonian to solve the problem of fermion doubling, with a Wilson term, and this procedure removes the spatial doublers as well as the the temporal ones for Wilson's

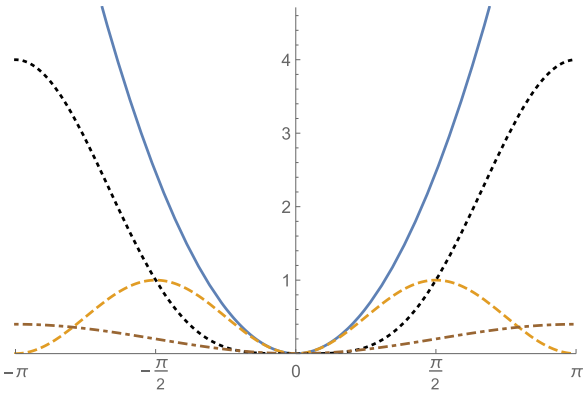

FIG. 4. The blue, solid curve shows $(f^{\mathrm{Dirac}}(k))^2$, the gold, dashed curve shows $(f^{\mathrm{naive}}(k))^2$, the black, dotted curve shows the noncrossed term $g^{\mathrm{noncrossed}}(k)$, and the brown, dot-dashed curve shows the crossed term $g^{\mathrm{crossed}}(k)$. We see that the biggest contribution to the fixing of the fermion doubling comes from the noncrossed term (with respect to the crossed term). That being said, any of the two terms is actually sufficient on its own to fix the doubling problem.

choice, $r = 1$ [30]. Here, however, we will stick to a Hamiltonian formulation and treat only spatial doublers. This is because in this paper the scheme is formulated in a Hamiltonian way. To treat temporal doublers in the two-step scheme of this paper, one would have to modify the original, DQW scheme.

b. Treatment of spatial doublers in the naive continuous-time scheme, via Wilson fermions

In order to treat the problem of spatial doublers in continuous time, described in Appendix B 4, we consider the following Hamiltonian [27]:

$$h^{\mathrm{LGT}} := h^{\mathrm{naive}} + h^{\mathrm{Schrö.}}, \tag{B36}$$

where

$$h^{\mathrm{naive}} := \alpha^1 \left(-i \frac{\mathcal{D}_1}{a} \right) + m\alpha^0 \tag{B37}$$

is the naive-discretization Hamiltonian considered in Appendix B 4 and

$$h^{\mathrm{Schrö.}} := \alpha^0 \frac{r}{a}(-\mathcal{L}) \tag{B38}$$

is the Wilson term, whose spatial operator, $\mathcal{L}/a$, is a discrete Laplacian [43],

$$\mathcal{L} = \mathcal{T}_1^{-1} + \mathcal{T}_1 - 2. \tag{B39}$$

Let us notice that the Laplacian is the spatial operator that intervenes in the nonrelativistic Schrödinger equation, hence the superscript "Schrö.".

The dispersion relation is now, plotted under the form of a gapless frequency,

$$\boxed{f^{\mathrm{LGT}}(k) := \sqrt{(\omega_{\pm}^{\mathrm{LGT}})^2 - m^2} = \sqrt{\frac{\sin^2(ka)}{a^2} + \left[m + \frac{r}{a}(1 - \cos(ka)) \right]^2 - m^2}.} \tag{B40}$$

In the left panel of Fig. 3, we see that the doubling problem is fixed with this expression, since there are no more poles at $-\pi/a$ and π/a. To develop explanations, it is practical to consider the square of the previous expression,

$$(f^{\mathrm{LGT}}(k))^2 = g^{\mathrm{naive}}(k) + g^{\mathrm{noncrossed}}(k) + g^{\mathrm{crossed}}(k), \tag{B41}$$

where

$$g^{\mathrm{naive}}(k) := \frac{\sin^2(ka)}{a^2} = (f^{\mathrm{naive}}(k))^2, \tag{B42a}$$

$$g^{\mathrm{noncrossed}}(k) := \frac{r^2}{a^2}(1 - \cos(ka))^2, \tag{B42b}$$

$$g^{\mathrm{crossed}}(k) := 2m\frac{r}{a}(1 - \cos(ka)). \tag{B42c}$$

Let us develop this expression, Eq. (B41), at next-to-next-to-lowest order in a,

$$\boxed{(f^{\mathrm{LGT}}(k))^2 = (1 + amr)k^2 + \left(\frac{1}{4}a^2r^2 - \frac{2}{3!}a^2 \right)k^4.} \tag{B43}$$

In Fig. 4, we see that the biggest contribution in fixing the doubling problem comes from the noncrossed term; this is actually also visible in the left panel of Fig. 3. That being said, any of the two terms is actually sufficient on its own to fix the doubling problem. Moreover, we see in Eq. (B43) that the crossed term unfortunately adds a first-order correction (in the lattice spacing) to the initial slope, that is, the latter becomes $1 + amr$ instead of 1, which is visible in the right panel of Fig. 3. Now, one can actually make this crossed term disappear, by choosing in the Wilson term $h^{\mathrm{Schrö.}}$, Eq. (B38), the operator α^2 instead of α^0. While in continuous time this has no impact on the unitarity of the scheme, it *will a priori* have an impact in discrete time [30], so this replacement cannot be made carelessly.

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[36] We take the liberty to consider σ as convenient; here, it is a set of indices, i.e., an unordered family. In practice, we will often order its elements, i.e., we will consider a list rather than a set.

[37] The question that one may ask oneself is whether there exists a "physical" h that is both linear and Hermitian but that does not lead to an undulatory phenomenology.

[38] We have identified k with the singlet $\{k\}$.

[39] Pay attention to the fact that although we use the notation $\hat{k}$, on the lattice, $\hat{k}$ and the position operator $\hat{x}$ do not satisfy the canonical commutation relations.

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[41] The present scheme is indeed not unitary in the following sense. Recall first that the unitarity of the two-step scheme in this paper has the following meaning: The two-step scheme is equivalent to the one-step scheme, for which the unitarity meaning is clear, provided that $\Psi_{j=1} = \mathcal{U}\Psi_{j=0}$. In the present case, endowing the naive two-step scheme with the same unitarity meaning does not yield a unitary one-step scheme.

[42] We here speak of the momentum of the discrete model, i.e., the product ϵk.

[43] This discrete Laplacian has been obtained by replacing $a\partial_1^2$ by $\mathcal{L} \equiv d_1^* d_1$, where d_1 and d_1^* are a forwards and a backwards finite difference, respectively (let us notice that they commute).