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# Path-integral solution of the one-dimensional Dirac quantum cellular automaton

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ABSTRACT

Quantum cellular automata, which describe the discrete and exactly causal unitary evolution of a lattice of quantum systems, have been recently considered as a fundamental approach to quantum field theory and a linear automaton for the Dirac equation in one dimension has been derived. In the linear case a quantum cellular automaton is isomorphic to a quantum walk and its evolution is conveniently formulated in terms of transition matrices. The semigroup structure of the matrices leads to a new kind of discrete path-integral, different from the well known Feynman checkerboard one, that is solved analytically in terms of Jacobi polynomials of the arbitrary mass parameter.



## 1. Introduction

The simplest example of discrete evolution of physical systems is that of a particle moving on a lattice. A (classical) *random walk* is exactly the description of a particle that moves in discrete time steps and with certain probabilities from one lattice position to the neighboring positions. This is a special instance of a *cellular automaton*, a more general discrete dynamical model introduced by von Neumann [1].

A quantum version of the random walk, called *quantum walk* (QW), was first introduced in [2] where a measurement of the $z$-component of a spin-$1/2$ particle decides whether the particle moves to the right or to the left. Later the measurement was replaced by a unitary operator on the spin-$1/2$ quantum system, also denoted internal degree of freedom or *coin* system, with the QW representing a discrete unitary evolution of a particle with internal degree of freedom given by the spin [3]. In the most general case the internal degree of freedom at a site $x$ of the lattice corresponds to a Hilbert space $\mathcal{H}_x$, and the total Hilbert space of the system is the direct sum $\bigoplus_x \mathcal{H}_x$ encompassing the Hilbert spaces of all the sites. As in the classical scenario, a QW is a special case of a *quantum cellular automaton* (QCA) [4], with cells of quantum systems locally interacting with a finite number of neighboring cells via a unitary operator. While QWs provide the one-step free evolution of one-particle quantum states, QCAs can describe the evolution of an arbitrary number of particles on the same lattice. However, replacing the quantum state with a quantum field on the lattice, a QW describes a QCA that is linear in the field (providing the discrete evolution of non-interacting particles with a given statistics). This corresponds to a "second quantization" of the QW and can ultimately be regarded as a QCA. This is what we call field QCA in the present paper.

Both QCAs and QWs have been a subject of investigation in computer-science and quantum information, where the two notions have been extensively studied and mathematically formalized (see Refs. [5–7,3,8,9]). The interest in these models was also motivated by the use of QWs in designing efficient quantum algorithms [10–13].

In Ref. [3] Ambainis et al. provided two general ideas for analyzing the evolution of a walk. The first idea consists in studying the walk in the momentum space, providing both exact analytical solutions and approximate solutions in the asymptotic limit of very long time. The second idea is to use the discrete path-integral approach, expressing the QW transition amplitude to a given site as a combinatorial sum over all possible paths leading to that site. Ref. [3] provides a path-sum solution of the *Hadamard walk* (the Hadamard unitary is the operator on the coin system), while Ref. [31] gives the solution for the *coined* QW, with an arbitrary unitary acting on the coin space. The same author considered the path-integral formulation for *disordered* QWs [32] where the coin unitary is a varying function of time.

The first attempt to mimic the Feynman path-integral in a discrete physical context is the Feynman *checkerboard problem* [14] that consists in finding a simple rule to represent the quantum

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dynamics of a Dirac particle in $1+1$ dimensions as a discrete path-integral. In Ref. [15] Kaufmann and Noyes simplify previous approaches [16,17] to the Feynman checkerboard, providing a solution of the finite-difference Dirac equation for a fixed value of the mass. However, such finite-difference equations have no corresponding QW or QCA, and generally lead to non-unitary evolutions. More recently, following the pioneering papers [18–20], a discrete model of dynamics for a relativistic particle has been considered in a QWs scenario [21–30].

Here we consider the unique automaton in one space dimension that satisfies the following basic principles: unitarity, linearity, locality, homogeneity and invariance with respect to the symmetries of the lattice. In Refs. [25,26] it has been shown that these constraints lead to a specific automaton model which describes the evolution of a quantum field with two internal degrees of freedom. Such a field automaton, which does not correspond to a coined QW, gives the usual Dirac equation in the relativistic limit of small wave-vectors where the lattice step is hypothetically assumed to be the Planck length. After reviewing the one dimensional Dirac automaton and the physical significance of its solutions, we solve analytically the automaton in the position space via a discrete path-integral, providing a discrete version of the Feynman propagator. In this formulation the discrete paths correspond to a sequence of the automaton transition matrices, which are proved to be closed under multiplication. Exploiting this feature, and the binary encoding of the admissible paths between two causally connected sites, we derive the analytical solution for an arbitrary initial state and mass parameter.

## 2. The one-dimensional Dirac QCA

The Dirac QCA of Refs. [25,26] describes the one-step evolution of a two-component quantum field

$$\psi(x,t) := \begin{pmatrix} \psi_R(x,t) \\ \psi_L(x,t) \end{pmatrix}, \quad (x,t) \in \mathbb{Z}^2,$$

$\psi_R$ and $\psi_L$ denoting the *right* and the *left* mode of the field. Here we restrict to one-particle states and the statistics is not relevant, but the presented solution could be extended to multi-particle state for any statistics consistent with the evolution. In the single-particle Hilbert space $\mathbb{C}^2 \otimes l_2(\mathbb{Z})$, we will use the factorized basis $|s\rangle|x\rangle$, with $s = R, L$.

Here the evolution of the field is restricted to be linear, namely there exists a unitary operator $A$ such that the one step evolution of the field is given by $\psi(t+1) = U\psi(t)U^\dagger = A\psi(t)$. In the present case the assumption of locality corresponds to writing $\psi(x,t+1)$ as linear a combination of $\psi(x+l,t)$ with $l = 0, \pm 1$. Homogeneity (or translation invariance) corresponds to a unitary operator $A$ of the form

$$\begin{aligned} &A = A_R \otimes T + A_L \otimes T^{-1} + A_F \otimes I, \\ &A_R = \begin{pmatrix} n & 0 \\ 0 & 0 \end{pmatrix}, \quad A_L = \begin{pmatrix} 0 & 0 \\ 0 & n \end{pmatrix}, \quad A_F = \begin{pmatrix} 0 & im \\ im & 0 \end{pmatrix}, \\ &T = \sum_{x\in\mathbb{Z}} |x+1\rangle\langle x|, \end{aligned} \tag{1}$$

where $A_R$, $A_L$, $A_F$ are called *transition matrices*, and $n^2 + m^2 = 1$, $n, m \in \mathbb{R}^+$.

The specific form of the transition matrices in Eq. (1) has been derived in Refs. [25,26] as a consequence of the constraints of unitarity and invariance with respect to the symmetries of the lattice, and the dynamics of the automaton (1) has been rigorously analyzed in the $k$ wave-vector space. Interpreting the parameter $k$ and $m$ of the Dirac automaton as momentum and mass it has been shown that the usual kinematics of the Dirac equation is recovered for small momenta ($k \to 0$) and small mass ($m \to 0$). The Dirac limit of the automaton is not proved taking a sequence of automata with smaller and smaller lattice and time spacing, i.e. the continuum limit given by lattice spacings and the time steps sent to 0, but rather fixing the automaton and computing the evolution of a class of states with limited band in momentum. For these states the automaton dynamics and the usual dynamics of the Dirac equation turn out to be indistinguishable.

It is worth noticing that the discrete model of evolution provided by the automaton (1) differs with respect to the one at the basis of the Feynman checkerboard. Indeed the checkerboard solutions to the Dirac equation are valid for discrete physics using finite differences calculus (where one usually recovers solutions to the infinitesimal Dirac equation in the appropriate continuous limit). On the other hand the automaton dynamics does not corresponds to a finite difference Hamiltonian or Lagrangian but to a discrete and exactly causal unitary evolution. The difference is even more clear observing that it does not exist a QCA whose evolution exactly corresponds to the finite difference Dirac differential equation. For these reasons the path-sum formulation of the Dirac QCA presented in the following does not coincide with the Feynman checkerboard one (see for example [15]) and it is based on the algebraic features of the transition matrices in Eq. (1).

## 3. Path-sum formulation of the Dirac QCA

Given the field initial condition $\psi(0)$, after $t$ time steps one has $\psi(t) = A^t\psi(0)$, and by linearity the field $\psi(x,t)$ must be a linear combination of the field at the points $(y,0)$ lying in the past causal cone of $(x,t)$. In general each point $(y,0)$ is connected to $(x,t)$ in $t$ time steps via a number of different discrete paths. According to Eq. (1) at each step of the automaton the local field $\psi(y,0)$ undergoes a shift $T^l$, $l = 0, \pm 1$, and the internal degree of freedom is multiplied by the corresponding transition matrix $A_h$, with $h \in \{R, L, F\}$. A generic path $\sigma$ connecting $x$ to $y$ in $t$ steps is conveniently identified with a string $\sigma = h_t h_{t-1} \ldots h_1$ of transitions, corresponding to the overall transition matrix given by the product

$$\mathcal{A}(\sigma) = A_{h_t} A_{h_{t-1}} \ldots A_{h_1}. \tag{2}$$

Summing over all admissible path $\sigma$ and over all points $(y,0)$ in the past causal cone of $(x,t)$, one has

$$\psi(x,t) = \sum_y \sum_\sigma \mathcal{A}(\sigma)\psi(y,0). \tag{3}$$

We now evaluate analytically the sum over $\sigma$ in Eq. (3) as a function of the variables $x$, $y$, $t$.

Upon denoting by $r$, $l$, $f$ the numbers of $R$, $L$, $F$ transitions in $\sigma$, using $t = r + l + f$ and $x - y = r - l$, one has

$$r = \frac{t - f + x - y}{2}, \qquad l = \frac{t - f - x + y}{2}. \tag{4}$$

The overall transition matrix $\sum_\sigma \mathcal{A}(\sigma)$ in (2) can be efficiently computed taking the following binary encoding

$$A_R = nA_{00}, \qquad A_L = nA_{11}, \qquad A_F = im(A_{10} + A_{10}) \tag{5}$$

$$A_{00} = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \qquad A_{11} = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \tag{6}$$

$$A_{01} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \qquad A_{10} = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \tag{7}$$

and observing that the matrices $A_{ab}$ satisfy the simple composition rule

$$A_{ab}A_{cd} = \frac{1+(-1)^{b\oplus c}}{2}A_{ad}, \tag{8}$$

$\oplus$ denoting the sum modulo 2. It is then convenient to denote by $\sigma_f = h_t, \dots h_1$ the generic path having $f$ occurrences of the $F$-transition, and write Eq. (3) as follows

$$\psi(x,t) = \sum_y \sum_{f=0}^{t-|x-y|} \sum_{\sigma_f} \mathcal{A}(\sigma)\psi(y,0). \tag{9}$$

In a path $\sigma_f$ the $F$ transitions identify $f+1$ slots

$$\tau_1 F \tau_2 F \dots\dots F \tau_{f+1}, \tag{10}$$

where $\tau_i$ denotes a (possibly empty) string of $R$ and $L$. According to Eq. (8) the generic path $\sigma$ cannot contain substrings of the form

$$h_i h_{i-1} = RL, \qquad h_i h_{i-1} = LR, \tag{11}$$

$$h_i h_{i-1} h_{i-2} = RFR, \qquad h_i h_{i-1} h_{i-2} = LFL, \tag{12}$$

since they give null transition amplitude. Therefore, according to Eq. (11) each $\tau_i$ in (10) is a string of equal letters, i.e. $\tau_i = hh\dots h$, with $h = R, L$. On the other hand Eq. (12) shows that two consecutive strings $\tau_i$ and $\tau_{i+1}$ must be made of different $h$. This corresponds to have all $\tau_{2i} = hh\dots h$ and all $\tau_{2i+1} = h'h'\dots h'$, with $h \neq h'$. In the following we will denote by $\Omega_R$ and $\Omega_L$ the sets of strings having $\tau_{2i+1} = RR\dots R$ and $\tau_{2i+1} = LL\dots L$, respectively, for all $i$.

The above structure for strings $\sigma_f$ can be exploited to determine the matrix $\mathcal{A}(\sigma_f)$. We consider separately the cases of $f$ even and $f$ odd. For $f$ even one has

$$\mathcal{A}(\sigma_f) = \alpha(f)\begin{cases} A_{00} + A_{11}, & f = t \\ A_{00}, & f < t,\ \sigma_f \in \Omega_R, \\ A_{11}, & f < t,\ \sigma_f \in \Omega_L, \end{cases} \tag{13}$$

while for $f$ odd one has

$$\mathcal{A}(\sigma_f) = \alpha(f)\begin{cases} A_{10} + A_{01}, & f = t \\ A_{10}, & f < t,\ \sigma_f \in \Omega_R, \\ A_{01}, & f < t,\ \sigma_f \in \Omega_L, \end{cases} \tag{14}$$

with the factor $\alpha(f)$ given by

$$\alpha(f) := (\mathrm{i}m)^f n^{t-f}. \tag{15}$$

According to Eqs. (13) and (14) we can finally restate Eq. (9) as

$$\psi(x,t) = \sum_y \sum_{a,b\in\{0,1\}} \sum_{f=0}^{t-|x-y|} c_{ab}(f)\alpha(f)A_{ab}\psi(y,0), \tag{16}$$

where $c_{aa}(2k+1) = c_{01}(2k) = c_{10}(2k) = 0$. The coefficients $c_{ab}(f)$ count the number of paths $\sigma_f$ which give $A_{ab}$ as total transition matrix, and are given by the following product of binomial coefficients

$$c_{ab}(f) = \binom{\mu_+ - \nu}{\frac{f-1}{2} - \nu}\binom{\mu_- + \nu}{\frac{f-1}{2} + \nu},$$
$$\nu = \frac{ab - \bar{a}\bar{b}}{2}, \qquad \mu_\pm = \frac{t \pm (x-y) - 1}{2}, \tag{17}$$

where $\bar{c} := c \oplus 1$, and the binomials are null for non-integer arguments. The expression of $c_{ab}$ is computed via combinatorial considerations based on the structure (10) of the paths, and on Eqs. (13) and (14). Let us start with the coefficients $c_{00}$ and $c_{11}$. The matrices $A_{00}$ and $A_{11}$ appear only for $f$ even (see Eq. (13)) in which case one has $\frac{f+2}{2}$ odd strings $\tau_{2i+1}$ and $\frac{f}{2}$ even strings $\tau_{2i}$. $A_{00}$ appears whenever $\sigma_f \in \Omega_R$, namely when the $R$-transitions are arranged in the strings $\tau_{2i+1}$. This means that we have to count in how many ways the $r$ identical characters $R$ and $l$ identical characters $L$ can be arranged in $\frac{f+2}{2}$ and $\frac{f}{2}$ strings, respectively. These arrangements can be viewed as combinations with repetitions which give

$$c_{00}(f) = \binom{\frac{f}{2}+r}{r}\binom{\frac{f}{2}+l-1}{l} = \binom{\frac{t+x-y}{2}}{\frac{f}{2}}\binom{\frac{t-x+y}{2}-1}{\frac{f}{2}-1},$$

where the second equality trivially follows from Eq. (4). Similarly $A_{11}$ appears whenever $\sigma_f \in \Omega_L$ which gives

$$c_{11}(f) = \binom{\frac{f}{2}+l}{l}\binom{\frac{f}{2}+r-1}{r} = \binom{\frac{t-x+y}{2}}{\frac{f}{2}}\binom{\frac{t+x-y}{2}-1}{\frac{f}{2}-1}.$$

Consider now the other two coefficients $c_{10}$ and $c_{01}$ counting the occurrences of $A_{10}$ and $A_{01}$. The last ones appears only when $f$ is odd (see Eq. (13)) and then one has the same number $\frac{f+1}{2}$ of odd strings $\tau_{2i+1}$ and even strings $\tau_{2i}$. Counting the combinations with repetitions as in the previous cases we get

$$c_{10}(f) = c_{01}(f) = \binom{\frac{f-1}{2}+r}{r}\binom{\frac{f-1}{2}+l}{l}$$
$$= \binom{\frac{t+x-y-1}{2}}{\frac{f-1}{2}}\binom{\frac{t-x+y-1}{2}}{\frac{f-1}{2}},$$

which concludes the derivation of the coefficients $c_{ab}(f)$ in Eq. (17).

The analytical solution of the Dirac automaton can also be expressed in terms of Jacobi polynomials $P_k^{(\zeta,\rho)}$ computing the sum over $f$ in Eq. (16)

$$\psi(x,t) = \sum_y \sum_{a,b\in\{0,1\}} \gamma_{a,b} P_k^{(1,-t)}\left(1 + 2\left(\frac{m}{n}\right)^2\right) A_{ab}\psi(y,0),$$
$$k = \mu_+ - \frac{a\oplus b + 1}{2},$$
$$\gamma_{a,b} = -(\mathrm{i}^{a\oplus b})n^t \left(\frac{m}{n}\right)^{2+a\oplus b} \frac{k!(\mu_{(-)^{ab}} + \frac{\overline{a\oplus b}}{2})}{(2)_k}, \tag{18}$$

where $\gamma_{00} = \gamma_{11} = 0$ ($\gamma_{10} = \gamma_{01} = 0$) for $t+x-y$ odd (even) and $(x)_k = x(x+1)\cdots(x+k-1)$.

## 4. Conclusions

We studied the one dimensional Dirac automaton, considering a discrete path-integral formulation. The analytical solution of the automaton evolution has been derived, adding a relevant case to the set of quantum automata solved in one space dimension, including only the coined QW and the disordered coined QW. The main novelty of this work is the technique used in the derivation of the analytical solution, based on the closure under multiplication of the automaton transition matrices. This approach can be extended to automata in higher space dimension. For example the transition matrices of the Weyl and Dirac QCAs in 2+1 and 3+1 dimensions recently derived in Ref. [26] enjoy the closure feature and their path-sum formulation could lead to the first analytically solved example in dimension higher than one.

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