Asymptotic properties of the Dirac quantum cellular automaton

A Pérez
Departament de Física Teòrica and IFIC,
Universitat de València-CSIC,
Dr. Moliner 50, 46100-Burjassot, Valencia
Spain

We show that the Dirac quantum cellular automaton [Ann. Phys. 354 (2015) 244] shares many properties in common with the discrete-time quantum walk. These similarities can be exploited to redefine the automaton as a unitary process that takes place at regular time steps on a one-dimensional lattice with an arbitrary lattice spacing. In this way, it becomes an alternative to the quantum walk, with a dispersion relation that can be controlled by a mass parameter, playing a similar role to the coin angle in the quantum walk. Moreover, the Dirac Hamiltonian is recovered under a suitable limit. We also provide two independent analytical approximations to the long term probability distribution. It is shown that, starting from localized conditions, the asymptotic value of the entropy of entanglement between internal and motional degrees of freedom overcomes the known limit that is approached by the quantum walk for the same initial conditions, and are similar to the ones achieved by highly localized states of the Dirac equation.

I. INTRODUCTION

The connection between physical processes on a lattice and the corresponding theories in the continuum is intriguing and plagued with difficulties and new features [1–3]. Discretization of quantum field theories that are defined on the continuum can be regarded as a powerful calculation tool, a paradigmatic example being QCD on a lattice [4], that allows for non perturbative calculations, after a suitable extrapolation is made to the limit of vanishing lattice spacing. In the case of fermion fields, one encounters problems like the “fermion doubling”, which can be attacked in different ways. This clearly shows that the discretization procedure of quantum field theories is not uniquely defined, with different approaches leading to the same limit in the continuum. In particular, this is true for the Dirac equation, which describes the relativistic motion of a spin 1/2 particle, and gives rise to interesting phenomena as the Zitterbewegung or the Klein paradox [5].

A recent paper [6] introduces a Dirac Quantum Cellular Automaton (DQCA), that describes the dynamics of a spin 1/2 particle on a one-dimensional lattice based on some symmetry principles. The model works as a set of updating rules on discrete space-time coordinates, where the time step and lattice spacing are to be identified with the Planck time $\tau_P$ and Planck length $l_P$, respectively. In the limit of large wavelengths (as compared to $l_P$) and small masses $m \ll m_P$, with $m_P$ the Planck mass, the Hamiltonian representing the DQCA approximates the Dirac Hamiltonian. The model also accounts for the above mentioned Zitterbewegung and Klein paradox phenomena [7].

Also interesting is the fact that the evolution of the probability distribution [6] resembles the one of a discrete time Quantum Walk (QW). The QW is the quantum analogue of the classical random walk. As in the case of random walks, QW’s can appear either under its discrete-time [8] or continuous-time [9] form. Moreover, it has been shown that any quantum algorithm can be recast under the form of a QW on a certain graph: QWs can be used for universal quantum computation, this being provable for both the continuous [10] and the discrete version [11]. Several experimental setups have been already performed to implement the QW [12–25].

In addition to the probability distribution, one immediately finds that the dispersion relation of the QW can be mapped into the one corresponding to the DQCA. Last, but not least, both models reproduce the Dirac equation in some limit, a property that has been established by several authors in the case of the QW [26–29]. These similarities suggest that the two models may share other properties that are worth studying. This is precisely the motivation of this paper. As we show, the DQCA can be reformulated as a unitary process taking place at regular time intervals $\tau$ on a lattice with arbitrary spacing $a$, thus providing an alternative to the QW, with some subtleties that will be discussed in detail, once the long term evolution has been derived. In this way, we establish a link between a model motivated from a lattice field theory, on the one side, and a process (the QW) that plays an important role in the theory of quantum information.

This paper is organized as follows. In Sect. II we review the general properties of the DQCA and the QW. We redefine the DQCA as a discrete time unitary process taking place on a one-dimensional lattice with arbitrary spacing. The dispersion relations of both models are discussed in Sect. III, and we show that the Dirac Hamiltonian is obtained from a suitable limit of the DQCA unitary operator. The similarities and differences of the probability distributions for both models are analyzed in Sect. IV. In Sect. V, we derive two different approximations to the long term probability distribution of the DQCA: We first obtain a simple formula from the $r$-th moment of the position
operator at large time steps, which only describes the gross features of the probability distribution, although we can extract the correct analytical behavior of the standard deviation. We next obtain an approximate result with the help of the stationary phase method, which turns out to work remarkably well, and correctly describes the details of the oscillations in the probability. Sect. VI is devoted to the study of the entanglement between the spatial and internal degrees of freedom, as quantified by the entropy of entanglement. We will show that, for a localized initial condition, this magnitude saturates the allowed maximum value for a two-dimensional Hilbert space, at variance with the lower limiting value which is approached by the QW for the same initial conditions. We discuss the similarity of the obtained result with highly localized initial states for the Dirac equation.

II. GENERAL PROPERTIES OF THE DQCA AND THE QW

A. QW

The standard QW corresponds to the discrete (both in time and in space) evolution of a one-dimensional quantum system (the walker) in a direction which depends on an additional degree of freedom, the chirality, with two possible states: “left” \(|L\) or “right” \(|R\). The global Hilbert space of the system is the tensor product \(H_L \otimes H_R\). \(H_L\) is the Hilbert space associated to the motion on the line, and it is spanned by the basis \(|x = na\rangle : n \in \mathbb{Z}\rangle\), where \(a\) is the lattice spacing, usually taken as the unit length. \(H_c\) is the chirality (or coin) Hilbert space, defined as a two-dimensional space that may correspond, for example, to a spin 1/2 particle, or to a 2-level energy system. Let us call \(T_-\) (\(T_+\)) the operators in \(H_c\) that move the walker one site to the left (right), and \(|L\rangle \langle L|, |R\rangle \langle R|\) the chirality projector operators in \(H_c\). We consider the unitary transformation

\[
U_{\text{QW}} = \{T_- \otimes |L\rangle \langle L| + T_+ \otimes |R\rangle \langle R|\} \circ \{I \otimes C(\theta)\},
\]

where \(C(\theta)\) is the coin operator, which acts only on the coin space. Any \(SU(2)\) matrix can be used but, for our purposes, it is sufficient to parametrize

\[
C(\theta) = \begin{pmatrix}
\cos \theta & -\sin \theta \\
\sin \theta & \cos \theta
\end{pmatrix},
\]

with \(\theta \in [0, \pi/2]\) a parameter defining the bias of the coin toss, \(I\) the identity operator in \(H_c\), and \(\sigma_i : i = x, y, z\) the Pauli matrices acting on \(H_c\). The effect of the unitary operator \(U_{\text{QW}}\) on the state of the system in one time step \(\tau\) is \(|\psi(t + \tau)\rangle = U_{\text{QW}}|\psi(t)\rangle\). The state vector can be expressed as

\[
|\psi(t)\rangle = \sum_{n=-\infty}^{\infty} |na\rangle \otimes [a_n(t) \langle R| + b_n(t) \langle L|].
\]

From the above we obtain

\[
|\psi(n, t)\rangle \equiv \langle na|\psi(t)\rangle = a_n(t) \langle R| + b_n(t) \langle L|
\]

or, in vector notation \(|\psi(n, t)\rangle = (a_n(t), b_n(t))^T\). At any given time step, the probability distribution of the walker can be calculated from

\[
P(n, t) = |a_n(t)|^2 + |b_n(t)|^2.
\]

B. DQCA

As mentioned in the Introduction, the Dirac Quantum Cellular Automaton is an extension of the Dirac field theory to the Planck and ultrarelativistic scales \([6,7]\). The model is defined by the repeated action of a unitary operator \(U_{DA}\) that acts on a spinor field \(\psi(x, t)\) with two internal degrees of freedom on a one-dimensional lattice with spacing \(l_P\) at time intervals \(\tau_P\), \(l_P\) and \(\tau_P\) being the Planck length and Planck time, respectively. In other words, \(x = nl_P, t = k\tau_P\) with \(n, k \in \mathbb{Z}\). The state \(|\psi(t + \tau_P)\rangle\) of the system at time \(t + \tau_P\) is related to the one at time \(t\) by

\[
|\psi(t + \tau_P)\rangle = U_{DA}|\psi(t)\rangle.
\]

If we represent the two internal degrees of freedom by \(|R\rangle, |L\rangle\), as in the QW, then using similar steps we can define

\[
|\psi(x, t)\rangle = (x|\psi(t)\rangle = \psi_R(x, t) |R\rangle + \psi_L(x, t) |L\rangle,
\]

where \(\psi_R(x, t)\) and \(\psi_L(x, t)\) are the components of the spinor field in the right and left states, respectively.
where $\psi_R(x,t)$ and $\psi_L(x,t)$ are the right and left spinor components of $|\psi(x,t)\rangle$, respectively. In vector notation, $\psi(x,t) = (\psi_R(x,t), \psi_L(x,t))^T$.

Starting from the hypothesis of unitarity, homogeneity of the interaction topology, invariance under time reversal and parity, and minimal dimension for a non-identical evolution, one arrives to the following form for the unitary operator:

$$U_{DA} = \alpha \{ T_- \otimes |L\rangle\langle L| + T_+ \otimes |R\rangle\langle R| \} - i\beta \sigma_z. \quad (8)$$

The constants $\alpha$ and $\beta$ can be taken as real numbers that satisfy the condition $\alpha^2 + \beta^2 = 1$ for $U_{DA}$ to be unitary.

Similarly to the QW, we can define the spatial probability distribution as

$$P(n,t) = |\psi_R(na,t)|^2 + |\psi_L(na,t)|^2. \quad (9)$$

We want to establish a connection between both models. To this purpose, we redefine the original DQCA as a unitary operation taking place on a lattice with arbitrary spacing $a$ at regular time steps $\tau$. In other words, we replace

$$l_p \to a, \quad \tau_p \to \tau, \quad (10)$$

and define

$$\beta \equiv \frac{mac}{\hbar}, \quad (11)$$

with $m$ a parameter that can be identified, in some limit, with the mass of the particle, as will be discussed below.

We notice that the last term in Eq. (8) only acts on the internal degrees of freedom, and does not include any displacement on the lattice. As we show later, this introduces some characteristic features on the evolution of the DQCA which are at variance with the QW.

### III. DISPERSION RELATION

Most properties of the QW are better analyzed by switching to the quasi-momentum space [30]. We introduce the basis of states $\{|p\rangle, p \in [-\pi \hbar/a, \pi \hbar/a]\}$ defined by

$$|p\rangle = \sqrt{\frac{a}{2\pi \hbar}} \sum_{n=-\infty}^{\infty} e^{ipna/\hbar} |na\rangle. \quad (12)$$

The unitary operators that govern both the QW and the DQCA become diagonal in this basis. We represent these operators by $U_{QW}(p)$ and $U_{DA}(p)$, respectively. Furthermore, the internal indices can be expressed in the $\{|R\rangle, |L\rangle\}$ basis. With these notations, we obtain

$$U_{QW}(p) = \begin{pmatrix} e^{-ipa/\hbar} & 0 \\ 0 & e^{ipa/\hbar} \end{pmatrix} C(\theta), \quad (13)$$

and

$$U_{DA}(p) = \begin{pmatrix} \alpha e^{-ipa/\hbar} & -i\beta \\ -i\beta & \alpha e^{ipa/\hbar} \end{pmatrix}. \quad (14)$$

In both cases, the eigenvalues can be written as $\eta_\pm(p) \equiv e^{-i\lambda(p)}$, $\eta_\pm(p) \equiv e^{i\lambda(p)}$, where $\lambda(p)$ satisfies the dispersion relation

$$\cos \lambda(p) = \cos \theta \cos(pa/\hbar), \quad (15)$$

for the QW, and

$$\cos \lambda(p) = \sqrt{1 - \left(\frac{mac}{\hbar}\right)^2 \cos(pa/\hbar)}, \quad (16)$$

in the case of the DQCA. Therefore, both dispersion relations take the same form, provided that we identify

$$\cos \theta \leftrightarrow \sqrt{1 - \left(\frac{mac}{\hbar}\right)^2}. \quad (17)$$
Figure 1: (Color online) Left panel: Probability distribution after $t = 200$ time steps for the QW, where only even sites are plotted. The initial state is localized at the origin, see Eq. (21). Middle panel: Distribution for the DQCA, with all sites showed (red dashed line), compared with the long-term approximation, Eq. (31) (black solid line). The right panel shows the differences for a smaller ($t = 10$) time step, where one clearly sees that the probability of the QW vanishes at odd sites of the lattice.

Many features of the time evolution can be obtained directly from the dispersion relation, such as the ballistic or diffusive behavior of the wave packet spreading [31], or the design of desired asymptotic probability distributions in one [32] or more dimensions [33].

From the unitary operator Eq. (14) one can extract the corresponding Hamiltonian, similarly to [6]. We first write $t = l\tau$, where $l \in \mathbb{N}$, and $\tau$ is the time step. We then define the Hamiltonian $H(p)$ by

$$U_{DA}^{l\tau}(p) \equiv \exp[-i\tau lH(p)].$$

(18)

Following this definition, one finds

$$H(p) = \frac{\hbar\lambda(p)}{\tau \sin \lambda(p)} \left( \begin{array}{cc} \alpha \sin(pa/\hbar) & \beta \\ -\alpha \sin(pa/\hbar) & \beta \end{array} \right).$$

(19)

One can recover the Dirac Hamiltonian in the limit $pa/\hbar \ll 1$, $mac/\hbar \ll 1$. In this limit, we have $\sin \lambda(p) \approx \lambda(p)$, $\sin(pa/\hbar) \approx pa/\hbar$ and $\alpha \approx 1$, so that

$$H(p) \approx \frac{a}{c\tau} \left( \begin{array}{cc} pc & mc^2 \\ mc^2 & -pc \end{array} \right).$$

(20)

By choosing the time step and the lattice spacing such that $\tau = a/c$, one obtains the Dirac Hamiltonian, where $m$ can be identified as the mass of the particle. The latter condition is a reminder of the original model, where $a = l_P$ and $\tau = \tau_P$, obviously related by $\tau_P = l_P/c$. In our proposal, these two parameters are no longer related to the Planck scale, but the Dirac dynamics can be recovered within the above restrictions.

IV. PROBABILITY DISTRIBUTION

In spite of sharing a common dispersion relation, both models will differ in several other aspects. For our analysis, we will fix some of the parameters appearing in these models. The QW will be studied using $\theta = \pi/4$ in (2), a choice that can be mapped to the standard Hadamard coin. As for the DQCA, the choice of units $c = \hbar = 1$ becomes appropriate. Moreover, we adopt the convention $a = 1$: In this way, we can label the site states as $|n\rangle$ in both cases. To allow a comparison with the QW on an equal footing, as discussed in the previous section, we will use the value $m = 1/\sqrt{2}$ for the following plots.

We first study the probability distribution, as defined in Eqs. (5) and (9). Figure 1 shows both probability distributions after $t = 200$ time steps, starting from the initial localized condition

$$\psi(n,0) = \frac{1}{\sqrt{2}} \left( \begin{array}{c} 1 \\ i \end{array} \right) \delta_{n,0}.$$  

(21)

One observes clear differences: The QW shows its characteristic peaks and a flat distribution in the middle, whereas the DQCA features more complicated structures. As it is well known, the probability distribution of the QW vanishes at odd (even) sites of the lattice when $t$ is even (odd). This is not true for the DQCA, as observed for $t = 10$ on the
same time steps. In fact, this is what Fig. (2) shows, where we plot the standard deviation $\sigma(t)$ as a function of $t$: After a few time steps, we obtain the characteristic ballistic $\sigma(t) \propto t$ spreading of the QW in both cases.

V. ASYMPTOTIC PROPERTIES

From the previous section it becomes apparent that, like in the QW case, we can expect well defined properties for the DQCA at large time steps. In fact, there are several methods to analytically derive the long term behavior of the probability distribution.

I) We first make use the method developed in [34] to obtain the convergence of the $r$-th moment

$$
E(x^r, t) \equiv \langle \psi(t) \mid x^r \mid \psi(t) \rangle,
$$

with $x$ the position operator. Inserting the resolution of the identity in the basis of $\{|p\}\}$ states (12) one obtains

$$
E(x^r, t) = \int_{-\pi}^{\pi} dp \langle \psi(p, t) \mid (i \frac{d}{dp} )^r \mid \psi(p, t) \rangle,
$$

where $|\psi(p, t)\rangle = \langle p \mid \psi(t)\rangle$ is a two-component spinor in quasi-momentum space. Using the unitary operator (14) in this basis, we can write

$$
|\psi(p, t)\rangle = U_{DA}^t(p)|\psi(p, 0)\rangle.
$$

The $t$-th power of $U_{DA}(p)$ is obtained from the spectral theorem:

$$
U_{DA}^t(p) = \sum_{s=\pm 1} e^{-i s \lambda(p) t} |\phi_s(p)\rangle \langle \phi_s(p)|.
$$

In the latter equation, $\lambda(p)$ is obtained from the dispersion equation (16), and $|\phi_s(p)\rangle, s = \pm 1$ are the two normalized eigenvectors of $U_{DA}(p)$, given by [6]:

$$
|\phi_s(p)\rangle = \frac{1}{\sqrt{2}} \left( \sqrt{1 + sv(p)} \right) / s \sqrt{1 - sv(p)} \right),
$$

where $v(p) = \frac{d}{dp} \sqrt{1 - m^2 \sin(p)/\sin \lambda(p)}$ is the group velocity that arises from (16). Using Eqs. (24) and (25), one arrives to the following relation

$$
\langle \psi(p, t) \mid (i \frac{d}{dp})^r \mid \psi(p, t) \rangle = (t)_r \sum_{s=\pm 1} \left( \frac{\eta'_s(p)}{\eta_s(p)} \right)^r \langle \phi_s(p) \mid \psi(p, 0) \rangle |^2 + O(t^{-1}).
$$

In the latter equation $\eta'_s(p)$ indicates the derivative with respect to $p$, and $(t)_r \equiv t(t-1) \cdots (t-r+1)$. After dividing by $t^r$ and taking the limit $t \rightarrow \infty$, one obtains

$$
\lim_{t \rightarrow \infty} E(x^r/t^r, t) = \sum_{s=\pm 1} \int_{-\pi}^{\pi} dp \left( \frac{\eta'_s(p)}{\eta_s(p)} \right)^r \langle \phi_s(p) \mid \psi(p, 0) \rangle |^2.
$$

Figure 2: (Color online) Standard deviation $\sigma(t)$ as a function of the time step $t$ for the QW (blue solid line), and for the DQCA (red dashed line). The initial state is localized at the origin, as in the previous figure.

Apart from these differences, the figure indicates that both probabilities spread equally with time, at least for large time steps. In fact, this is what Fig. 2 shows, where we plot the standard deviation $\sigma(t)$ as a function of $t$: After a few time steps, we obtain the characteristic ballistic $\sigma(t) \propto t$ spreading of the QW in both cases.
Let us work out the above expression for the initial localized state Eq. (21), for which $|\psi(p,0)\rangle = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} a \\ b \end{pmatrix}$. In this case, one finds $\langle \phi_s(p) | \psi(p,0) \rangle^2 = 1/4\pi$, both for $s = 1$ and $s = -1$. On the other hand, we can write $\frac{\eta_0^\dagger(p)}{\eta_0(p)} = sv(p)$, so that Eq. (28) becomes

$$\lim_{t \to \infty} E(x'/t',t) = \frac{1}{4\pi} \int_{-\pi}^{\pi} dp \ [v^\prime(p) + (-v(p))^\prime].$$

(29)

We next change the integration variable in the first term of the latter expression by inverting the function $y = v(p)$. Similarly, we perform the transformation $y = -v(p)$ on the second term. After some algebra, we arrive to the final expression

$$\lim_{t \to \infty} E(x'/t',t) = \frac{1}{\pi} \int_{-\sqrt{1-m^2}}^{\sqrt{1-m^2}} dy \ p'(y)y',$$

(30)

with the notation $p'(y) \equiv \frac{m}{(1-y^2)\sqrt{1-m^2-y^2}}$. Eq. (30) implies that the variable $x/t$ is distributed across the interval $[-\sqrt{1-m^2}, \sqrt{1-m^2}]$ with a probability distribution given by

$$P(y) = \frac{1}{\pi} p'(y) \equiv \frac{m/\pi}{(1-y^2)\sqrt{1-m^2-y^2}}.$$

(31)

As shown in Fig. 1, our result Eq. (31) provides a simple approximation to the actual probability distribution of the DQCA, although it does not reproduce the oscillations seen on the true evolution. However, it can be used to obtain the standard deviation at large time steps, as this magnitude does not depend on the details of the distribution. By taking $r = 2$ in Eq. (30), one obtains

$$\sigma(t) = t\sqrt{1-m},$$

(32)

which accounts for the ballistic spreading observed in Sect. IV. Indeed, the previous result was expected from the similarity of the dispersion relations of the QW (see [31]) and the DQCA.

II) A better approximation to the long-time asymptotic distribution can be obtained following the stationary phase method. Let us consider a localized initial condition, such that

$$|\psi(p,0)\rangle = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} a \\ b \end{pmatrix},$$

(33)

and $|a|^2 + |b|^2 = 1$. Making use of Eqs. (24), (25) and (26), we arrive to $|\psi(p,0)\rangle = (\psi_R(p,t), \psi_L(p,t))^T$, where

$$\psi_R(p,t) = \frac{1}{\sqrt{2\pi}} |a \cos \lambda(p)t - ia v(p) \sin \lambda(p)t - ib \sqrt{1 - v^2(p)} \sin \lambda(p)t|$$

(34)

$$\psi_L(p,t) = \frac{1}{\sqrt{2\pi}} |b \cos \lambda(p)t + ib v(p) \sin \lambda(p)t - ia \sqrt{1 - v^2(p)} \sin \lambda(p)t|.$$  

(35)

The corresponding spinor in position space is obtained from

$$\psi_{R,L}(n,t) = \int_{-\pi}^{\pi} \frac{dp}{\sqrt{2\pi}} e^{ipn} \psi_{R,L}(p,t).$$

(36)

Let us introduce the notations $\alpha = n/t$, $I_1(\alpha, t) = \int_{-\pi}^{\pi} \frac{dp}{2\pi} e^{-i\lambda(p)t}g_1(p)$, with $g_1(p) = 1$, $g_2(p) = v(p)$, and $g_3(p) = \sqrt{1 - v^2(p)}$. Then, the above result can be written as

$$\psi_R(n,t) = a\Re \{I_1(\alpha, t)\} - a\Im \{I_2(\alpha, t)\} - ib\Im \{I_3(\alpha, t)\}$$

(37)

$$\psi_L(n,t) = b\Re \{I_1(\alpha, t)\} + b\Re \{I_2(\alpha, t)\} - ia\Im \{I_3(\alpha, t)\}.$$  

(38)
Our goal is to obtain an approximation to the integrals $I_i(\alpha, t)$, with $g_i(p)$ a smooth function satisfying $g_i(-p) = g_i(p)$, which implies that $I_i(-\alpha, t) = I_i(\alpha, t)$. We make use of the stationary phase method, and consider the phase $\Phi(p, \alpha) = \lambda(p) + \alpha p$ appearing in these integrals. One needs to look for the roots $p_i(\alpha), i = 1, 2 \ldots$ of the equation

$$\frac{\partial \Phi(p, \alpha)}{\partial p} = v(p) + \alpha = 0,$$

and expand $\Phi(p, \alpha)$ around $p_i(\alpha)$:

$$\Phi(p, \alpha) \simeq \Phi(p_i(\alpha), \alpha) + \frac{1}{2}(p - p_i(\alpha))^2\lambda''(p_i(\alpha)).$$

Let us first assume $\alpha > 0$. After careful inspection, we obtain the roots $p_1(\alpha) = -p_s$, and $p_2(\alpha) = \pi + p_s$, where $p_s \equiv \arccos \sqrt{(1 - m^2 - \alpha^2)/(1 - \alpha^2)}$. For the first solution, one needs to replace $\lambda(p) \rightarrow \lambda(p_s) \equiv \lambda_s$, $\lambda''(p) \rightarrow \lambda''(p_s) = \sqrt{1 - m^2 - \alpha^2(1 - \alpha^2)/m} \geq 0$, while for the second solution we have to use $\lambda(p) \rightarrow \pi + \lambda_s$, $\lambda''(p) \rightarrow -\lambda''(p_s)$.

After substitution into the definition of $I_i(\alpha, t)$ and integration, we obtain the following approximation

$$I_i(\alpha, t) \simeq \frac{1}{\sqrt{2\pi t\lambda''(p_s)}}[g_i(-p_s)e^{it\phi(\alpha)+i\pi/4} + g_i(\pi + p_s)e^{it(\alpha\pi - \phi(\alpha)+\pi)-i\pi/4}],$$

where $\phi(\alpha) = \lambda_s - |\alpha|p_s$, the above expression being valid for $|\alpha| \leq \sqrt{1 - m^2}$. In particular, the above formula gives

$$I_1(\alpha, t) \simeq \frac{1}{\sqrt{2\pi t\lambda''(p_s)}}[e^{it\phi(\alpha)+i\pi/4} + e^{it(\alpha\pi - \phi(\alpha)+\pi)-i\pi/4}],$$

To obtain $I_2(\alpha, t)$ we make use of condition (39). It then follows $I_2(\alpha, t) \simeq -\alpha I_1(\alpha, t)$. Following a similar argument, we arrive to $I_3(\alpha, t) \simeq \sqrt{1 - \alpha^2}I_1(\alpha, t)$. In order to test the accuracy of the above approximations, we have represented in Fig. 3 the probability distribution for the DQCA, as obtained from the stationary phase method, compared with the exact evolution, starting from the localized initial condition Eq. (33) with $a = 1, b = i$. The plot shows that this approximation works extremely well, and accurately describes the oscillatory behavior of the probability within the limits $|\alpha| \leq \sqrt{1 - m^2}$.

The details of these oscillations are better seen for a simple case, corresponding to the initial condition

$$\psi(n, 0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}\delta_{n,0}.$$

For this particular case the probability distribution can be expressed, after some algebra, as

$$P(\alpha, t) = \frac{1}{\pi t \lambda''(p_s)} \left\{(1 + \alpha)^2[1 + (-1)^{t+\alpha}] \cos^2(t\phi(\alpha) + \pi/4) + (1 - \alpha^2)[1 - (-1)^{t+\alpha}] \sin^2(t\phi(\alpha) + \pi/4)\right\}.$$
VI. ENTANGLEMENT

A characteristic property of the QW is that entanglement between the coin and spatial degrees of freedom is generated as a consequence of the evolution \[35\]. The amount of entanglement is usually quantified using the von Neumann entropy of the reduced density matrix of the coin degrees of freedom, after tracing out the spatial ones. More precisely, we define this quantity, as a function of the time step \(t\), by

\[
S(t) = -\text{Tr} \left\{ \rho_c(t) \log_2 \rho_c(t) \right\},
\]

where \(\rho_c(t) = \sum_n \langle n | \psi(t) \rangle \langle \psi(t) | n \rangle\) is the reduced density matrix for the coin space, \(\text{Tr}\) represents the trace operation in this space, and \(\log_2\) is the logarithm in base 2.

As numerically obtained by the above authors, and proven later in \[36\], for a Hadamard walk with localized initial conditions the asymptotic entanglement is \(S_{\text{lim}} \approx 0.8720\) for all initial coin states, although higher values can be reached by starting from non-localized conditions (see also \[37\]). An obvious question to ask is whether the DQCA is also limited to this amount of entanglement, when the evolution starts from the same state. Fig. (4) plots the entropy of entanglement \(S(t)\) as a function of the time step for both the QW and the DQCA. We immediately see that, for the QW, one approaches the predicted value \(S_{\text{lim}}\). Interestingly, the DQCA model overcomes this value, and reaches the allowed maximum \(S_{\text{max}} = 1\) for a 2-dimensional system, thus indicating that internal and motion degrees of freedom become maximally entangled. Such large values of the entanglement are also reached for the one-dimensional Dirac equation with narrow initial conditions, for some configurations of the internal degrees of freedom, including the one used in Eq. \[21\] \[27\]. When considering highly localized states for the Dirac equation, one has to be careful, since arbitrarily peaked states are inconsistent with the one-particle approach \[38\]. One can, however, consistently restrict to positive (or negative) energy eigenvalues. For such states, the evolution of highly localized wave packets gives rise to maximal entanglement.

VII. CONCLUSIONS

The connection of field theories on a lattice with simpler models that can be used, in some limit, to simulate those theories, has proven to be both a useful computational tool, and an avenue towards the understanding of the underlying difficulties of the initial system. In this work, we have investigated the time evolution of the Dirac Quantum Cellular Automaton, initially proposed as a discretized version that accounts for the motion of a relativistic spin 1/2
particle in one dimension [6], and compared its properties with those of the Quantum Walk, an important primitive for quantum information. The probability distribution looks similar for both systems, with some differences which arise from the fact that the DQCA includes a term in the probability amplitude that forces the walker to stay at the original position, at variance with the known properties of the QW. In spite of these differences, both probability distributions propagate in a similar manner, as clearly shown by the close resemblance of the standard deviation in both cases.

We have given two analytic approximations to the probability distribution at large time steps. The first one was obtained by calculating the generalized momentum of the position operator. In this way, one obtains a simple result that only describes the general shape of the distribution, although it suffices to take account for the observed ballistic evolution of the standard deviation. On the other hand, the stationary phase method provides a remarkable approximation, and clearly shows the effect of the above mentioned “probability to stay” term in the DQCA.

The analysis of the entanglement between the internal and spatial degrees of freedom reveals that the DQCA approaches a maximally entangled state when the initial condition is a localized state at one point of the lattice. This result clearly overcomes the known limiting values of the QW for similar initial conditions. Maximally entangled states also appear for some localized solutions of the Dirac equation in the continuum so that, in this respect, the DQCA looks closer to a Dirac particle than the QW.

To summarize, the DQCA can be regarded as an alternative to the QW, which shares many properties with it, while possessing some new distinctive features. At the same time, given its original motivation, it can easily serve as a model to illustrate many properties of the Dirac equation, such as the Zitterbewegung and scattering from a potential [7].

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