Quantum Cellular Automata Models for General Dirac Equation

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Abstract

The goal of this study is to provide an exact unitary quantum cellular automata that, under discrete time steps, converges towards the Generalized Dirac Equation (GDE) in the continuum limit. The evolutionary rules for such a single particle walk are discussed in this paper, and it is shown that this quantum cellular automata will maintain similar properties to the GDE. Index terms— quantum, random, walk, dirac, gas, lattice

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1 Introduction

Quantum cellular automata provide an efficient method for computational use. While classically, computational methods such as randomized search have been used for a variety of algorithms, quantum random walks may be exploited for quantum computational tasks. There is vast literature on the significant speedups due to quantum
random walks and the application of complex amplitudes rather than normal probability, see [4].

With the advent of quantum computers, quantum random walks can be extended into applications of computation. For instance, one may find a speedup using a quantum random walk along a graph in solving the graph search problem [2] while the well known quantum Grover search algorithm is very similar to a random walk algorithm, in finding an element of a set. The overall advantages of these algorithms are based on the fact that quantum walks may operate using many states randomly, as opposed to the limited bit-wise states that classical computation is restricted to. Quantum random may also be used in algorithmic simulation of certain quantum mechanical equations.

For each cell, there is an evolution of its complex probability amplitude affecting adjacent cells; the evolution must be unitary for the sum of the norms squared of the amplitudes to add to 1. Earlier studies have been on non-unitary processes, where after an evolution, the probability amplitudes were re-normalized to maintain sum over probabilities equal to 1, but these were only approximate simulations, accumulating errors at each time step.

Examples of simple Quantum Random Walks are numerous; these include the Uniform Walk, Hadamard Walk [12], Walks on Honeycomb lattices [15], etc.

The Dirac equation, in particular, describes the natural motion of a spin - 1/2 particle; a generalized Dirac equation also exists as a solution to the Klein-Gordon wave equation. Previous studies have made a quantum cellular automata model for the Dirac equation [1] and [5], but none have been made for the generalized equation. The reasoning for these studies is that the Dirac Equation occurs more naturally as a quantum phenomenon in terms of quantum walks, and perhaps can exhibit better practicality with quantum algorithms. Note that however, unlike regular automata in which every cell has the exact same process, the Dirac equation is 2-vector valued, and does not have symmetric evolutionary rules, but instead, is different based on direction and the negative and positive signs for each entry in the vector.

It is worth noting that extension of the 2-vector case to a 4-directional case in (2+1) dimensions cannot preserve probability, while in the the case of (3+1) dimensions [16], the 3-d Dirac equation with a 8-vector representation does simulate accurately.

Here, we present a proof of a unitary, convergent QCA model for the Generalized Dirac Equation. We will show that it converges properly to the continuous setting. We will also note that the extra parameter from generalization affects the experimental result of spreading. Then we will prove that by eigen-decomposition and combinatorically, it will also converge towards a solution of the Generalized Dirac equation. Finally, we will show the interpretation of the mass and angle parameters in terms of simulation.

2 Quantum Random Walks

The following section provides the formalism for our study. Suppose that our space is a circular lattice, an approximation for the circular spaces in the literature that correspond to position by an angle in \([0, 2\pi]\):
2.1 Definition

Define a discrete Hilbert space with a set of orthonormal basis using Bra-ket vectors,

\[ |1\rangle, |2\rangle, \ldots, |n\rangle \tag{1} \]

where \(|i + n\rangle = |i\rangle\) because we are working on a periodic, circular lattice. Then every vector \(|\psi\rangle\) may be represented in terms of

\[ |\psi\rangle = \sum_{i=1}^{n} w_{i} |i\rangle \tag{2} \]

where \(w_{i} \in \mathbb{C}\). Then \(\langle \psi |\) is the complex conjugate of \(|\psi\rangle\), and the inner product is defined as the dot product \(\langle \psi | * |\psi\rangle\) This is also defined as a superposition of quantum states. Every linear evolution of \(\psi\) can be represented as the multiplication of a matrix \(M\), i.e.

\[ M |\psi_{1}\rangle = |\psi_{2}\rangle \tag{3} \]

Note that this is the analogue to a classical Markov Chain, but \(M\) does not satisfy the stochastic matrix condition. Rather, it must satisfy the unitary condition for the sum of the probabilities to be 1 i.e. \(M\overline{M} = I\)

3 Dirac Equation

Ignoring natural units, the Dirac equation is a natural solution of the Klein-Gordon Wave Equation, well known within quantum mechanics:

\[ (-\partial_{t}^{2} + \nabla^{2}) \psi = m^{2} \psi \tag{4} \]

where \(m\) is a constant mass term and the left hand side \(\Box = \partial^{2}t - \nabla^{2}\) is the wave operator.

One of the solutions to this equation is the Generalized Dirac equation, given by decomposition of the equation into two complex conjugate parts through operator calculus, and assuming \(\psi\) is a two-vector wavefunction:

\[ (\sigma_{2}\partial_{x} - i\sigma_{1}\partial_{t})\psi = m(\cos \rho \cdot I + i \sin \rho \cdot \sigma_{3})\psi \tag{5} \]

where \(\sigma_{i}\)'s are the Pauli matrices. Here, the difference is the inclusion of \(\rho\) into the equation: This allows an extra parameter for the random walk from which effects we will see later on.

From this, if we discretize the partial differentials, we get:

3.1 Generalized Dirac Equation Random Walk

In order to discretize (5), our random walk must satisfy two conditions:

1. Because the set of discrete steps is \(O(1/\epsilon)\), our random walk must only accumulate errors of order \(O(1/\epsilon^{2})\).

2. Such a random walk must satisfy the unitary property.
By applying finite differences on the partial differentials from (5), we may obtain the following equations:

\begin{align}
\psi_-(x,t+\epsilon) &= (\im \epsilon \cos \rho) \psi_+(x,t) + (\epsilon \sin \rho) \psi_+(x-\epsilon,t) + (\im \epsilon \rho_1) \psi_-(x,t) + (\epsilon \rho_2) \psi_-(x+\epsilon,t) \\
\psi_+(x,t+\epsilon) &= (\im \epsilon \cos \rho) \psi_-(x,t) - (\epsilon \sin \rho) \psi_-(x+\epsilon,t) - (\im \epsilon \rho_1) \psi_+(x,t) + (\epsilon \rho_2) \psi_+(x-\epsilon,t)
\end{align}

(6)

Note that the recursion, for the amplitudes on \( x \) at the next \( \epsilon \) time step depends on the states at \( x-\epsilon, x, x+\epsilon \). This generates a highly complicated dynamical system, in which a particle with for example, "-" spin can either move forward and change its spin to "+", stay stationary and change its spin to "+", or follow its spin. In order to simplify this, we show that at decreasing values of \( \epsilon \), that such a recursion will converge to a simpler and well known system, one in which particles cannot both move and change spin. The convergence will have \( O(\epsilon^2) \) error, which is acceptable.

If we make the reasonable assumption that \( \psi_+, \psi_- \) are differentiable functions, then we may use a first order approximation: \( \psi(x-\epsilon,t) = \psi(x,t) + O(\epsilon) \). Thus by taking the continuum limit,

\[
\lim_{\epsilon \to 0} (\epsilon \sin \rho) \psi_+(x-\epsilon,t) = (\epsilon \sin \rho) \psi_+(x,t) + O(\epsilon^2)
\]

(8)

A similar approach can easily be taken for \( \psi_- \) as well. The continuum limit will also give

\[
\lim_{\epsilon \to 0} \im \rho_1 \psi_-(x,t) + \rho_2 \psi_-(x-\epsilon,t) = \psi_-(x+\epsilon,t)
\]

(9)

\[
\lim_{\epsilon \to 0} -\im \rho_1 \psi_+(x,t) + \rho_2 \psi_+(x-\epsilon,t) = \psi_+(x-\epsilon,t)
\]

(10)

This follows the approach from [?], as normally, most random walks are of the form \( \psi(x,t+1) = a \cdot \psi(x,t-1) + b \cdot \psi(x,t+1) \). This naturally corresponds to a block diagonal matrix generated by a tensor, of the form \( \mathcal{H} = \mathcal{H}_p \otimes \mathcal{H}_s \), where \( \mathcal{H}_p \) corresponds to a translation action, and \( \mathcal{H}_s \) corresponds to the coefficients. Writing out the form explicitly gives us, from letting \( R = \epsilon \), we can let the transition matrix \( M \) be of the form:

\[
\begin{pmatrix}
\ldots \quad R \cdot \sin \rho & g_1 & i \cdot R \cdot \cos \rho & g_2 & 0 & \ldots \\
\ldots \quad f_2 & i \cdot R \cdot \cos \rho & f_1 & -R \cdot \sin \rho & 0 & \ldots \\
\ldots \quad 0 & R \cdot \sin \rho & g_1 & i \cdot R \cdot \cos \rho & g_2 & 0 & \ldots \\
\ldots \quad 0 & f_2 & i \cdot R \cdot \cos \rho & f_1 & -R \cdot \sin \rho & 0 & \ldots \\
\ldots \quad 0 & 0 & R \cdot \sin \rho & g_1 & i \cdot R \cdot \cos \rho & g_2 & 0 & \ldots \\
\ldots \quad 0 & 0 & f_2 & i \cdot R \cdot \cos \rho & f_1 & -R \cdot \sin \rho & 0 & \ldots \\
\ldots
\end{pmatrix}
\]
where $R, f_1, f_2, g_1, g_2$ are introduced as dummy variables. For the unitary condition, they must satisfy the following conditions:

\[
\begin{align*}
  g_1 \bar{g}_1 + g_2 \bar{g}_2 + R R \cos \rho \cos \rho + R R \sin \rho \sin \rho &= 1 \\
  -i f_1 R \cos \rho + f_2 R \sin \rho + i R \bar{g}_1 \cos \rho - R \bar{g}_2 \sin \rho &= 0 \\
  g_1 \bar{g}_2 - i R^2 \cos \rho \sin \rho &= 0 \\
  -i f_2 R \cos \rho + i R \bar{g}_2 \cos \rho &= 0 \\
  g_2 \bar{g}_1 + i R^2 \cos \rho \sin \rho &= 0 \\
  f_1 R \sin \rho - R \bar{g}_1 \sin \rho &= 0 \\
  -i g_1 R \cos \rho - g_2 R \sin \rho + i R \bar{f}_1 \cos \rho + R \bar{f}_2 \sin \rho &= 0 \\
  f_1 \bar{f}_1 + f_2 \bar{f}_2 + R R \cos \rho \cos \rho + R R \sin \rho \sin \rho &= 1
\end{align*}
\]

These equations may be simplified down to:

\[
\begin{align*}
  f_1 &= \bar{g}_1 \\
  f_2 &= \bar{g}_2 \\
  g_2 \bar{g}_1 &= -i R^2 \sin \rho \cos \rho \\
  |g_1|^2 + |g_2|^2 + R^2 &= 1
\end{align*}
\]

If we allow $g_1 = i r_1$ and $g_2 = r_2$, then we may obtain the following equations:

\[
\begin{align*}
  r_1 r_2 &= (m \epsilon)^2 \sin \rho \cos \rho \\
  r_1^2 + r_2^2 &= 1 - (m \epsilon)^2
\end{align*}
\]

Solving this quadratic will give us the following formulas for the variables. However, the walk must depend on the granularity parameter $\epsilon$. 

5
3.2 Simulations

Figures above with $(0.4, 0)$, $(0.4, \pi/6)$, $(0.8, 0)$
In the figures above, all walks were simulated with an initial condition of $(1/4, 1/4)$ amplitude, with the x-axis lattice being 100 points long, and with the y-axis representing time, up to 300 frames. From the figures above, all walks can be parametrized by a $(R, \rho)$ pair. A key difference is in the behavior of this walk due to the extra $\rho$ term, compared to the mass term.

This is effectively the simulation of a single particle. Note that $R$ in the simulation represents the mass term. As mass increases, the amplitude for a particle staying becomes higher, while the amplitudes for spreading decreases. It can be interpreted as an angular relation term. Furthermore, $\rho$ may represent the “spreading” term. Note the extreme difference between the simulations of $(0.8, 0.2)$ compared to $(0.8, \pi/6)$. The former maintains most of its amplitudes, as it travels in both directions. However, the latter spreads uniformly, although slowly. This suggests of course, as an extension, different parametrization may give significantly different results when using quantum random walks for certain problems.

Although the amplitude coefficients differ by negative signs, the simulation shows however, that the propagation is still approximately symmetric. The asymptotic behavior however, does not tend to high density probabilities. This evolution, as time $t$ tends to infinity will produce a roughly uniform distribution. As $\rho$ becomes higher, the spreading becomes much more apparent. In the case of $\rho = 0$, this is consistent with results found in [1].

We take note that in [18], simulations of these quantum random walks can be improved
using state-of-the-art scientific computational methods. So far we have shown that such a walk is both unitary and converges to the GDE by an error of $O(\epsilon^2)$. Now we look at the properties of such a walk.

### 3.3 Path Integral Approach

Note that there is an explicit combinatorial approach to solving the amplitude at a given location at a given time, which is consistent with using Feynman path integrals in the continuous case.

The two equations are not symmetric with respect to $+/-$; this is due to the non-symmetric Pauli matrices. It is possible to enumerate the paths with base 4 strings, with a function on the string to determine amplitude coefficients, but it is difficult to solve this combinatorically exactly. Such an approach would involve large casework and analysis of partition functions, whose simplified versions are covered in [1].

We can apply representation theory by exchanging the elements into matrices. The Dihedral group, denoted $D_n$, is the set of the $2n$ rotation and reflection symmetries of a $n$-sided polygon. Assuming we are orienting positive direction as clockwise, then let the group element $R_i$ denote rotation by $i$ units, while $S_i$ denotes rotation of $i$ units, then a reflection. Then geometrically, these properties must hold true:

$$
R_i R_j = R_{i+j}, \quad R_i S_j = S_{i+j}, \quad S_i R_j = S_{i-j}, \quad S_i S_j = R_{i-j}
$$

Note that using the group representation theory, then the elements are isomorphic to

$$
R_k = \begin{bmatrix}
\cos \frac{2\pi k}{n} & -\sin \frac{2\pi k}{n} \\
\sin \frac{2\pi k}{n} & \cos \frac{2\pi k}{n}
\end{bmatrix}, \quad S_k = \begin{bmatrix}
\cos \frac{2\pi k}{n} & \sin \frac{2\pi k}{n} \\
-\sin \frac{2\pi k}{n} & \cos \frac{2\pi k}{n}
\end{bmatrix}
$$

Now, define the generating function under this algebra:

$$
f(t) = (a_0 R_0 + a_1 R_1 + b_0 S_0 + b_1 S_1)^t \quad (14)
$$

We take note that we can allow $a_0, a_1, b_0, b_1$ to correspond to the coefficients from (6) and (7). As the terms multiply, it is not hard to see that biject to the particle moving using the evolution rules.

By calculation, one can find the mapping from $\mathbb{C}[D_n]$ to a direct isomorphic sum of $\text{End}(V_i)$, where $V_1, V_2, \ldots$ are the irreducible representations of $D_n$, which will then find the coefficients on $R_k$ and $S_k$ for any given $k$.

Because this is additive, any initial conditions may be solved with the same method. However, the precise combinatorial approach is also simply the expansion and cancellation of terms from diagonalization of the matrix $M$. Each probability amplitude may be expressed as the weighted sum of powers of eigenvalues, analogous to a Markov matrix process. Due to the norms of the eigenvalue being 1, the sum will tend to be cyclic as the power $t$ grows; this effectively simulates the wave-like evolution.

Unlike well-known expander graphs [17] with classical random walks, in which the convergence towards uniform distribution is based on the gap between the two largest eigenvalues, quantum random walks do not behave as such, and can easily vary between different unit-vector states, due to the eigenvalues of the transition matrix all being complex unit vectors.

For this case, the spectrum of the eigenvalues in the random walk matrix can be found in Appendix B.
4 Conclusion

We have shown successfully that there exists a quantum cellular automata model for the GDE. Furthermore, such a model is unitary, convergent with errors of $O(\epsilon^2)$, and its simulation brings up a question about the parametrization and pre-optimization involving quantum random walks, related to natural quantum processes such as the Dirac Equation. Some open questions, as mentioned in the introduction, will involve discretization of larger dimensional Dirac Equations, as well as non-linearities. So far, as the author only knows currently, only continuous versions of non-linear equations have been studied in [8].

5 Acknowledgements

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6 Appendix A: Quantum Random Walk Coding

\[ R = 0.8 \]
\[ p = 1 ; \]
\[ t = 300 ; \]
\[ n = 100 ; \]
\[ \text{array} = \text{Table}[\{0 , 0\} , \{i , t\} , \{j , n\}] ; \]
\[ \text{array}[[1]] [[n/2]] [[1]] = 1/4 ; \]
\[ \text{array}[[1]] [[n/2]] [[2]] = 1/4 ; \]
\[ \text{array}[[1]] [[n/2 + 1]] [[1]] = 1/4 ; \]
\[ \text{array}[[1]] [[n/2 + 1]] [[2]] = 1/4 ; \]
\[ S = \sqrt{R^2 + \text{Sin}[2 \cdot p]} ; \]
\[ r1 = S[[1]] ; \]
\[ r2 = S[[2]] ; \]
\[ e1 = \text{Conjugate}[g1] ; \]
\[ e2 = \text{Conjugate}[g2] ; \]
\[ \text{For}[a = 2 , a <= t , a++, \]
\[ \text{For}[b = 1 , b <= n , b++, \]
\[ \text{If}[b == 1 , \]
\[ \text{array}[[a]] [[b + 1]] [[2]] += N[g2] \cdot \text{array}[[a - 1]] [[b]] [[2]] ; \]
\[ \text{array}[[a]] [[b + 1]] [[1]] += N[R \cdot \text{Sin}[p]] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \text{array}[[a]] [[n]] [[2]] += N[-R \cdot \text{Sin}[p]] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \text{array}[[a]] [[n]] [[1]] += N[g2] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \]
\[ \text{If}[b == n , \]
\[ \text{array}[[a]] [[1]] [[2]] += N[f2] \cdot \text{array}[[a - 1]] [[b]] [[2]] ; \]
\[ \text{array}[[a]] [[1]] [[1]] += N[R \cdot \text{Sin}[p]] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \text{array}[[a]] [[b - 1]] [[2]] += N[-R \cdot \text{Sin}[p]] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \text{array}[[a]] [[b - 1]] [[1]] += N[g2] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \]
\[ \text{If}[b == n && b != 1 , \]
\[ \text{array}[[a]] [[b + 1]] [[2]] += N[f2] \cdot \text{array}[[a - 1]] [[b]] [[2]] ; \]
\[ \text{array}[[a]] [[b + 1]] [[1]] += N[R \cdot \text{Sin}[p]] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \text{array}[[a]] [[b - 1]] [[2]] += N[-R \cdot \text{Sin}[p]] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \text{array}[[a]] [[b - 1]] [[1]] += N[g2] \cdot \text{array}[[a - 1]] [[b]] [[1]] ; \]
\[ \]
\[ \text{array} [[n]] [[2]] = \text{Abs}[\text{array}[[s]] [[r]] [[1]] + \text{Abs}[\text{array}[[s]] [[r]] [[2]]] ; \]
\[ \text{array} [[n]] [[1]] = \text{Abs}[\text{array}[[s]] [[r]] [[1]] - \text{Abs}[\text{array}[[s]] [[r]] [[2]]] ; \]
\[ \]
\[ \text{EvolutionMatrix} = \text{Table}[\{0 , 0\} , \{i , t\} , \{j , n\}] ; \]
\[ \text{EvolutionMatrix}[[1]] [[i]] [[1]] [[1]] = 1/2 ; \]
\[ \text{EvolutionMatrix}[[1]] [[i]] [[2]] [[2]] = 1/2 ; \]
\[ \text{EvolutionMatrix}[[1]] [[i]] [[2]] [[1]] = N[R \cdot \text{Sin}[p]] ; \]
\[ \text{EvolutionMatrix}[[1]] [[i]] [[1]] [[2]] = 1/4 ; \]
\[ \text{EvolutionMatrix}[[1]] [[i]] [[1]] [[1]] = N[R \cdot r1] ; \]

7 Appendix B: Eigenvalues

\[ M = 1/4 ; \]
\[ p = 1 ; \]
\[ t = 3 ; \]
\[ n = 6 ; \]
\[ S = \sqrt{R^2 + \text{Sin}[2 \cdot p]} ; \]
\[ r1 = S[[1]] ; \]
\[ r2 = S[[2]] ; \]
\[ \text{EvolutionMatrix} = \text{Table}[\{0 , 0\} , \{i , n\}] ; \]
\[ \text{EvolutionMatrix}[[i]] [[i]] [[1]] [[1]] = N[R \cdot \text{Sin}[p]] ; \]
\[ \text{EvolutionMatrix}[[i]] [[i]] [[2]] [[2]] = N[R \cdot r2] ; \]
\[ \text{EvolutionMatrix}[[i]] [[i]] [[1]] [[2]] = 1/4 ; \]
\[ \text{EvolutionMatrix}[[i]] [[i]] [[2]] [[1]] = N[1 \cdot r1] ; \]
\[ \text{EvolutionMatrix}[[i]] [[i + 1]] [[i + 1]] = N[I \cdot \text{Sin}[p]] ; \]
\[ \text{EvolutionMatrix}[[i]] [[i + 1]] [[i + 2]] = N[I \cdot \text{Sin}[p]] ; \]
\[ \text{EvolutionMatrix}[[i]] [[i + 2]] [[i + 1]] = N[I \cdot r1] ; \]

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evolutionmatrix[[i + 1]][[i]][[1]][[2]] = N[r2];
evolutionmatrix[[i + 1]][[i]][[2]][[2]] = N[−R*Sin[p]];
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