

Discrete Time Quantum Walk on a Line with two Particles

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Abstract

We introduce the idea of a quantum walk with two particles and study it for the case of a discrete time walk on a line[1]. We consider both separable and maximally entangled initial conditions, and show how the entanglement and the relative phase between the states describing the *coin* degree of freedom of each particle will influence the evolution of the quantum walk. In particular, these factors will have consequences on the distance between the particles and the probability to find them in a given point, yielding results that cannot be obtained from a separable initial state, be it pure or mixed. Finally, we review briefly proposals for implementations.

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I. INTRODUCTION

Quantum walks, first proposed in 1993 [2], are the quantum analogue of classical random walks. Quantum walks have recently generated much interest (for an overview, see [3]), in particular because they are proving to be a very useful technique for the construction of quantum algorithms, just as random walks are for classical algorithms. In fact, several quantum algorithms based on quantum walks have been shown to be optimal [4, 5], and the only algorithm currently proven to offer an exponential speed-up with respect to its classical counterpart [6] is based on a (continuous time) quantum walk.

The crucial difference between quantum and random walks is that the former allow for quantum superpositions of the walker states and explore the interference of the terms in these superpositions. The resulting probability distributions after N steps are very different, as can be seen in Figure 1. Furthermore, a quantum walk exhibits a variance proportional to N , which represents a quadratic speed-up over the classical case, where the variance goes as \sqrt{N} .

II. THE MULTIPARTICLE WALK

The new concept being introduced in this paper is the idea of using multiple walkers — quantum particles — simultaneously in the same quantum walk. This idea has been used classically, where k walkers traversing the same graph are equivalent to k independent random walks. These additional resources can be used, for instance, to improve the time to hit a certain node of the graph. In the quantum case though, the multiple-walker situation becomes even more interesting, because the particles can be entangled, which results in final probability distributions which cannot be described by multiple independent single-particle walks. We will show that the entanglement in a quantum walk on a line can be tuned to cover more space.

III. THE QUANTUM WALK FORMALISM

Let us now describe a single-particle discrete time quantum walk on a line. A single step of the walk comprises two operations: the coin flip \hat{C} and the conditional shift \hat{S} . The coin degree of freedom is encoded by a qubit, whose states we will denote $|\uparrow\rangle$ and $|\downarrow\rangle$, and the

coin flip is a unitary operator that sets a basis state into a superposition over that basis. We have that $\hat{C} \in SU(2)$ acts on the coin Hilbert space \mathcal{H}_C . The most commonly used example is the Hadamard transformation, and we shall use this throughout as the coin:

$$\hat{H} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \quad (1)$$

This coin is said to be *unbiased* in the sense that an initial state $|\uparrow\rangle$ will be set into an equal superposition of “up” and “down”, $\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle)$, after being acted upon by the coin. This corresponds to equal probabilities of the particle being found in the state $|\uparrow\rangle$ or $|\downarrow\rangle$ if measured after one operation. The second part of a single step of the walk is the shift operation \hat{S} , acting on \mathcal{H}_P — the Hilbert space encoding the possible positions of a particle on an infinite discrete line. The basis vectors of \mathcal{H}_P will be denoted $|i\rangle$, where $i \in \mathbb{Z}$. Thus the total Hilbert space of the walk is given by:

$$\mathcal{H} = \mathcal{H}_C \otimes \mathcal{H}_P, \quad (2)$$

and the states of the quantum walk will be described by vectors in \mathcal{H} .

We will consider the following shift operator:

$$\hat{S} = \sum_i (|\uparrow\rangle \langle\uparrow| \otimes |i+1\rangle \langle i| + |\downarrow\rangle \langle\downarrow| \otimes |i-1\rangle \langle i|). \quad (3)$$

This has the effect of moving a particle in the “up” state one unit to the right and a particle in the “down” state one unit to the left. If the particle in question is in some superposition of “up” and “down”, the terms evolve accordingly. \hat{C} acts on the coin state space and \hat{S} acts on both the position state space and coin space together. The total operator for each step is unitary and will have the form:

$$\hat{U} = \hat{S}(\hat{I}_P \otimes \hat{C}). \quad (4)$$

where I_P is the identity operator on the position space. So, for example, if the initial state is $|\uparrow\rangle \otimes |0\rangle$, the first step of the walk gives:

$$\hat{U}(|\uparrow\rangle \otimes |0\rangle) = \frac{1}{\sqrt{2}}(|\uparrow\rangle \otimes |1\rangle + |\downarrow\rangle \otimes |-1\rangle). \quad (5)$$

If a measurement is performed at this point, then the walk agrees with its classical counterpart: there is a 50% probability of the particle being found at position +1 and a 50%

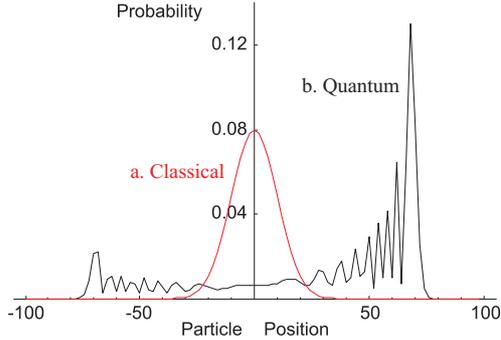


FIG. 1: Probability distributions for discrete time random walks on a line after $N = 100$ steps: (a) the classical walk, (b) the quantum walk with a Hadamard coin and initial state $|0\rangle \otimes |1\rangle$.

probability of the particle being found at position -1 . Yet, after the first two steps of the walk, the progression of the quantum and classical walks begin to diverge wildly. This becomes particularly clear after a few dozen steps. In Figure 1 we present the probability distributions for both the classical random walk and the quantum walk for $N = 100$.

Note that the quantum walk shows a relatively low probability associated with the walker being found close to the origin: rather, the peaks of the distribution correspond to the particle being found a considerable distance away. On the other hand, in the classical case, the origin is precisely the point where the probability for the particle to be found is maximal. There is a \sqrt{N} speed-up of the quantum walk over the classical in terms of expected deviation of the walker from the origin.

IV. QUANTUM WALK WITH TWO PARTICLES

Let us now generalize this definition of the discrete time quantum walk on a line to the case of two walkers. Consider two particles, 1 and 2, simultaneously completing quantum walks on the same line. Let the joint Hilbert space of the two-particles system be \mathcal{H}_{12} . Then, we have:

$$\mathcal{H}_{12} = \mathcal{H}_1 \otimes \mathcal{H}_2, \quad (6)$$

where \mathcal{H}_1 and \mathcal{H}_2 are the Hilbert spaces of particles 1 and 2 respectively. Both \mathcal{H}_1 and \mathcal{H}_2 are isomorphic to \mathcal{H} , as defined in Equation (2). Similarly, the new walk operator will be

\hat{U}_{12} , given by:

$$\hat{U}_{12} = \hat{U} \otimes \hat{U}. \quad (7)$$

Now suppose that two particles are set into the walk in a pure separable initial state, for example:

$$|\Psi_0^{sep}\rangle = |0, \downarrow\rangle_1 |0, \uparrow\rangle_2. \quad (8)$$

In this case, the two particles evolve throughout the walk simultaneously, but independently, so that after N steps:

$$|\Psi_N^{sep}\rangle = \hat{U}_{12}^N |\Psi_0^{sep}\rangle = \hat{U}^N |0, \downarrow\rangle_1 \hat{U}^N |0, \uparrow\rangle_2. \quad (9)$$

This is equivalent to two separate walks being completed on two different lines at the same time. The probability distributions are both identical (though one is inverted in the position coordinate relative to the other) and independent.

However, this is a quantum mechanical scheme, so it is also possible for a pair of particles to be set into the walk in a joint state which is entangled. For example, consider two maximally entangled states:

$$|\psi_0^\pm\rangle_{12} = \frac{1}{\sqrt{2}}(|0, \downarrow\rangle_1 |0, \uparrow\rangle_2 \pm |0, \uparrow\rangle_1 |0, \downarrow\rangle_2), \quad (10)$$

Note that these also describe the cases of a pair of identical particles on the same point, either bosons (the “+” state) or fermions (the “−” state). Now the evolution of the walk cannot be described as two separate walks progressing independently. The joint state of the particles’ evolution after N steps is:

$$|\psi_N^\pm\rangle_{12} = \hat{U}_{12}^N |\psi_0^\pm\rangle_{12} = \frac{1}{\sqrt{2}} \left(\hat{U}^N |0, \downarrow\rangle_1 \hat{U}^N |0, \uparrow\rangle_2 \pm \hat{U}^N |0, \uparrow\rangle_1 \hat{U}^N |0, \downarrow\rangle_2 \right). \quad (11)$$

These two scenarios correspond to very different final joint probability distributions. Let $P_{12}(i, j, N)$ denote a joint probability over the two particles of finding particle 1 in position i and particle 2 in position j after N steps of the walk. In the case of the separable initial conditions, $|\Psi_0^{sep}\rangle = |0, \downarrow\rangle_1 |0, \uparrow\rangle_2$,

$$P_{12}^{sep}(i, j; N) = P_1^{sep}(i; N) \times P_2^{sep}(j; N), \quad (12)$$

which is just the product of two independent distributions for single-particle walks after N steps. This is in agreement with the observation that the two particles in the walks

proceed independently, and without reference to each other, into the final state given in Equation (9). However, this equation does not describe the case of entangled particles, which have walk evolutions which depend on the existence of the other particle in the walk. The joint probability distribution must be symmetric under exchange of the labels 1 and 2 for the “+” case and, for the “-” case, the distribution must remain unchanged when *both* the labels of the particles are exchanged and the position axes are reflected. These distributions are presented graphically in Figure 2 for the case $N = 60$. Looking at the plots, it is clear that these distributions are significantly different.

In the case of the separable initial conditions, the plot in Figure 2.a is just the product of two distributions like the one in Figure 1.b. The initial state is $|\Psi_0^{sep}\rangle = |0, \downarrow\rangle_1 |0, \uparrow\rangle_2$, so the distribution for particle 2 is biased towards the right (as shown in Figure 1.b) and the distribution for particle 1 is biased towards the left — a mirror image of the distribution for particle 2. Figure 2.b shows the distribution for P_{12}^+ and Figure 2.c shows the distribution for P_{12}^- .

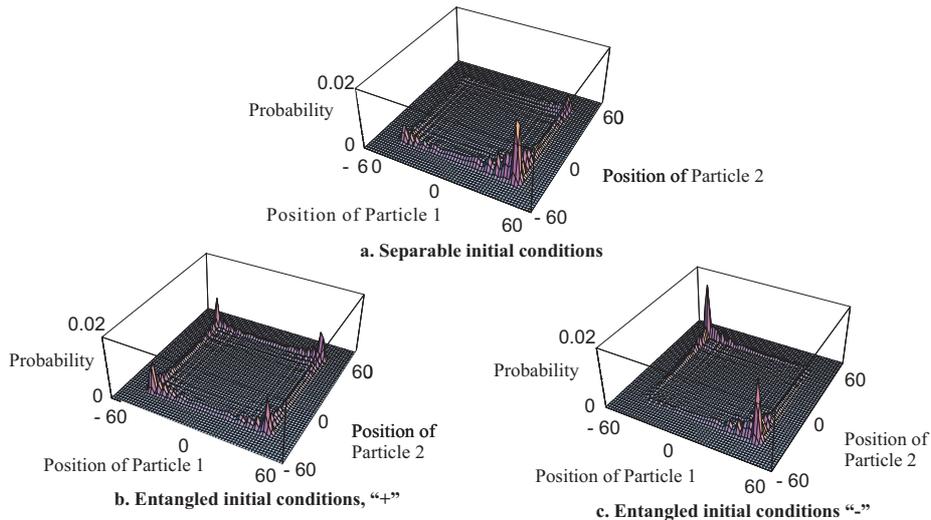


FIG. 2: Two-particles probability distributions after $N = 60$ steps for different initial conditions: (a) separable state $|\psi_0^S\rangle_{12}$; (b) $|\psi_0^+\rangle_{12}$ state; and (c) $|\psi_0^-\rangle_{12}$ state. Note that the peak of the distribution in (a) has been cropped.

In all three distributions the maxima occur around $i, j \simeq 42$, but the effect of the entanglement is dramatic. Entanglement can induce the walk to explore certain configurations with relatively high probability that in a walk beginning in a separable state would be very

unlikely. For example, the higher maxima of the distribution for the symmetric entangled state (“+” state) correspond to the particles being found on the same side of the origin and both near $|i|, |j| \simeq 42$. Conversely, in the antisymmetric, “-”, case, there are a whole set of configurations that have probability zero associated with their occurrence. These are the configurations along the line $i = j$, which implies that the two particles are never in the same position on the line. Note that a pair of identical fermions conducting a quantum walk will follow this distribution (Figure 2.c), in which the particles have high probability of being found at opposite ends of the line. A pair of identical bosons will follow the symmetric distribution shown in Figure 2.b.

The behaviors of the individual particles in the quantum walk for entangled initial conditions also exhibit interesting features. Tracing over the degrees of freedom of one of the particles leaves a reduced density matrix:

$$\rho_1 = \text{Tr}_2 (|\psi_N^\pm\rangle_{12} \langle \psi_N^\pm|_{12}) = \frac{1}{2} \hat{U}^N |0, \downarrow\rangle \langle 0, \downarrow| \hat{U}^{\dagger N} + \frac{1}{2} \hat{U}^N |0, \uparrow\rangle \langle 0, \uparrow| \hat{U}^{\dagger N}. \quad (13)$$

which is an equal mixture of the states $U^N |0, \downarrow\rangle$ and $U^N |0, \uparrow\rangle$. These are simply the evolution states after N steps for a walk starting from the state $|0, \downarrow\rangle$ and the state $|0, \uparrow\rangle$. Therefore the marginal probability distribution for finding one of the particles in position i after N steps is given by

$$P_1^\pm(i; N) = \frac{1}{2} [P_\downarrow(i; N) + P_\uparrow(i; N)] = P_2^\pm(i; N). \quad (14)$$

Note that $P_\downarrow(i; N)$ and $P_\uparrow(i; N)$ are the probability distributions of a single-particle walk initialized in the state $|0, \downarrow\rangle$ and $|0, \uparrow\rangle$. Again compare this situation to the case of separable states. The separable initial condition given in Equation (8) generates the marginal probability distributions $P_1^{sep}(i; N) = P_\downarrow(i; N)$ and $P_2^{sep}(i; N) = P_\uparrow(i; N)$, yielding a joint probability distribution which is just the product of these (Equation (12)). This is not the case for the entangled state, where the joint probability distribution contains information about the correlations between the positions of the two particles, which will become apparent on measurement of the two particles’ positions.

There are further joint properties of the two particles which are of interest. Let us define the distance $\Delta_{12}^{sep, \pm}$ between the two particles’ final (independently) measured positions, x_1 and x_2 , after N steps:

$$\Delta_{12}^{sep, \pm} \equiv |x_1 - x_2|, \quad (15)$$

where $x_1, x_2 \in [-N, \dots, 0, \dots, N]$. Table IV presents the expectation value of this distance for the three different initial conditions, and for different N . From this data, it is evident that the particles are more likely to remain closer together for the “+”-entangled initial conditions than for the separable initial state, and more likely to remain farther apart in the case of the “-”-entangled initial state than for the separable state. In fact, we can make a stronger statement than this; for a given N we always have:

$$\langle \Delta_{12}^- \rangle - \langle \Delta_{12}^{sep} \rangle = \langle \Delta_{12}^{sep} \rangle - \langle \Delta_{12}^+ \rangle \quad (16)$$

Let us now consider the correlation function between the spatial distribution of each of the two particles:

$$C^{sep,\pm}(x_1, x_2) \equiv \langle x_1 x_2 \rangle - \langle x_1 \rangle \langle x_2 \rangle. \quad (17)$$

Clearly, in the case of the separable initial condition (8), this correlation is always zero. For the other cases, the values of $C^\pm(x_1, x_2)$ are presented in Table IV for different N . Given the symmetry of the P_{12}^\pm distributions, we have that in those cases $\langle x_1 \rangle = \langle x_2 \rangle = 0$. Thus, the sign difference in the correlation function expresses the tendency for the two particles in the “-” case to end the quantum walk on different sides of the line (with respect to the origin, 0), and on the same side for the “+” case.

Finally, let us now calculate, for the different initial conditions, the probability of finding at least one particle in position i after N steps: $\mathcal{P}^{sep,\pm}(i; N)$. This is clearly a joint property as it depends on both one-particle outcomes:

$$\begin{aligned} \mathcal{P}^{sep,\pm}(i; N) &= \sum_{j=-N}^N [P_{12}^{sep,\pm}(i, j; N) + P_{12}^{sep,\pm}(j, i; N)] - P_{12}^{sep,\pm}(i, i; N) \\ &= [P_{\downarrow}(i; N) + P_{\uparrow}(i; N)] - P_{12}^{sep,\pm}(i, i; N). \end{aligned} \quad (18)$$

Given a one-particle probability distribution, say $P_{\downarrow}(i; N)$ [note that $P_{\uparrow}(i; N) = P_{\downarrow}(-i; N)$], our probability $\mathcal{P}^{sep,\pm}(i; N)$ decreases with the joint probability $P_{12}^{sep,\pm}(i, i; N)$ and is maximal in the “-” case, as we always have $P_{12}^-(i, i; N) = 0$. In fact, around the points (40, 40) and (-40, -40) in Figure IV we clearly have:

$$\mathcal{P}^-(i; N) > \mathcal{P}^{sep}(i; N) > \mathcal{P}^+(i; N). \quad (19)$$

We see that, by introducing entanglement in the initial conditions of our two-particles quantum walk, the probability of finding at least one particle in a particular position on the

Expectation value $\langle \Delta_{12}^{sep,\pm} \rangle$ after N steps						
Nb. of steps N	10	20	30	40	60	100
Init. cond. $ \psi_0^-\rangle_{12}$	8.8	17.5	26.0	34.9	52.2	87.0
Init. cond. $ \psi_0^{sep}\rangle_{12}$	7.1	14.7	21.9	29.5	44.3	73.9
Init. cond. $ \psi_0^+\rangle_{12}$	5.5	11.9	17.8	24.1	36.3	60.8

Correlation function $C^{sep,MS,\pm}(x_1, x_2)$ after N steps						
Nb. of steps N	10	20	30	40	60	100
Init. c. $ \psi_0^-\rangle_{12}$	-16.8	-69.8	-153.5	-276.2	-619.7	-1718.3
Init. c. $\hat{\rho}_{12}^{MS}(0)$	-6.0	-31.4	-70.6	-130.4	-299.3	-839.3
Init. c. $ \psi_0^{sep}\rangle_{12}$	0	0	0	0	0	0
Init. c. $ \psi_0^+\rangle_{12}$	4.8	7.3	13.7	15.1	23.1	39.1

line can actually be better or worst than in the case where the two particles are independent. Note that in this case this does not depend on the particular amount of entanglement introduced, as both states in Equation (10) are maximally entangled, but rather on their symmetry/relative phase.

V. THE CASE OF MIXED INITIAL STATE

Now, we turn to the discussion of whether a separable state can achieve the same results as entangled ones. First, we note that the differences between the cases of entangled and separable initial states occur with respect to the joint (two-particles) properties, rather than individual ones. We will show that a mixed separable state diagonal in the $\{|0, \downarrow\rangle_1 |0, \uparrow\rangle_2, |0, \uparrow\rangle_1 |0, \downarrow\rangle_2\}$ basis cannot achieve the same values for the correlation function and the distance between the two particles as entangled states. Let us consider the following mixed state, a weighted mixture of two alternatives described by the states $|0, \downarrow\rangle_1 |0, \uparrow\rangle_2$ and $|0, \uparrow\rangle_1 |0, \downarrow\rangle_2$, as a new initial state for our two particles quantum walk:

$$\hat{\rho}_{12}^{MS}(0) = a|0, \downarrow\rangle\langle 0, \downarrow|_1 \otimes |0, \uparrow\rangle\langle 0, \uparrow|_2 + b|0, \uparrow\rangle\langle 0, \uparrow|_1 \otimes |0, \downarrow\rangle\langle 0, \downarrow|_2, \quad (20)$$

where $a, b \in \mathbb{R}^+$ such that $a + b = 1$. After N steps of the quantum walk, the system will be in the state $\hat{\rho}_{12}^{MS}(N) = \hat{U}^N \hat{\rho}_{12}^{MS}(0) \hat{U}^{\dagger N}$, and the marginal probability distributions will be:

$$\begin{aligned} P_1^{MS}(i; N) &= aP_{\downarrow}(i; N) + bP_{\uparrow}(i; N), \\ P_2^{MS}(i; N) &= aP_{\uparrow}(i; N) + bP_{\downarrow}(i; N). \end{aligned} \quad (21)$$

We see that in general ($a \neq b$) they are biased, and that:

$$\langle x_1 \rangle = \sum_{i=-N}^N iP_1^{MS}(i; N) = a\langle x_{\downarrow} \rangle + b\langle x_{\uparrow} \rangle = (a - b)\langle x_{\downarrow} \rangle = -\langle x_2 \rangle. \quad (22)$$

Here, we have used $\langle x_{\downarrow, \uparrow} \rangle \equiv \sum_{i=-N}^N iP_{\downarrow, \uparrow}(i; N)$, $P_{\downarrow, \uparrow}(i; N)$ being the probability distributions after N steps for initial states $|0, \downarrow\rangle$ and $|0, \uparrow\rangle$, and the fact that $\langle x_{\downarrow} \rangle = -\langle x_{\uparrow} \rangle$.

The joint probability distribution after N steps, as seen from Equation (20), is given by:

$$P_{12}^{MS}(i, j; N) = aP_{\downarrow}(i; N)P_{\uparrow}(j; N) + bP_{\uparrow}(i; N)P_{\downarrow}(j; N), \quad (23)$$

and is *not* the product of two one-particle marginal distributions $P_{\downarrow}(i; N)$ and $P_{\uparrow}(j; N)$. Our state $\hat{\rho}_{12}^{MS}(N)$ is separable, but it is also correlated. Its correlation function $C^{MS}(x_1, x_2)$ is not zero, as can clearly be seen from the definition of the correlation function (using $\langle x_1 x_2 \rangle = -\langle x_{\downarrow} \rangle^2$):

$$C^{MS}(x_1, x_2) \equiv \langle x_1 x_2 \rangle - \langle x_1 \rangle \langle x_2 \rangle = -[1 - (a - b)^2] \langle x_{\downarrow} \rangle^2 = 2ab \langle x_{\downarrow} \rangle^2. \quad (24)$$

In Table IV, we present the values of $C^{MS}(x_1, x_2)$ for the case $a = b = \frac{1}{2}$. As the function $[1 - (a - b)^2] \in [0, 1]$, we see that $\hat{\rho}_{12}^{MS}(N)$ is always less correlated than a singlet entangled state. Actually, $\hat{\rho}_{12}^{MS}(N)$ is only a *classically correlated* state, and when compared with entangled states $|\psi_N^{\pm}\rangle_{12}$, it exhibits the same features as the pure separable state $|\psi_N^{PS}\rangle_{12}$. Namely, the expectation value of the distance is the same for both pure and mixed separable states, $\langle \Delta_{12}^{MS} \rangle = \langle \Delta_{12}^{sep} \rangle$, as seen from the probability distribution (23). Similarly, we see that the probability of finding at least one particle in position i after N steps is the same for both pure separable and mixed separable case: $\mathcal{P}^{sep}(i; N) = \mathcal{P}^{MS}(i; N)$.

VI. CONCLUSIONS, FURTHER STUDY, AND IMPLEMENTATIONS

There are a number of natural extensions to our work on discrete time quantum walks on a line with two entangled particles, starting with the study of other initial entangled

states and the introduction of more particles. It would also be interesting to consider other graphs for the walks, as well as less standard coins, such as unbalanced or even entangling ones [8, 9]. Another direction worth exploring would be a multiparticle quantum walk in continuous time, which does not use a coin, and which could be a relevant model to study the evolution of dilute quantum gases. Finally, it would also be of great interest to explore our ideas for particular applications or the design of efficient quantum algorithms. Random walks have been employed in such tasks as estimating the volume of a convex body [10] and the connectivity in P2P networks [11]. Quantum walks could have an important contribution to these problems, in particular our proposal with two entangled particles, which can cover more space than two independent particles, as we saw for the “-” case.

There have been several proposals to implement a single-particle quantum walk, using cavity QED [12], optical lattices [13] and ion traps [14]. The latter could be adapted to the two particles case by encoding the coin states in the electronic levels of two ions and the position in their *com* or *stretch* motional modes: the coin flipping could then be obtained with a $\pi/2$ Raman pulse and the shift with a conditional optical dipole force [15]. Another possibility is to send two photons through a tree of balanced beam splitters which implement both the coin flipping and the conditional shift, again generalizing a scheme proposed for a single particle [8, 16]. Note that this could be implemented with other particles as well, e.g. electrons, using a device equivalent to a beam splitter [17]. Finally, we would like to point out that, by considering indistinguishable bosons or fermions, the effects of quantum statistics can be used to prepare the initial entangled states, thus appearing again as a resource for quantum information processing [18].

In this article we introduced the concept of a quantum walk with two particles and studied it for the case of a discrete time walk on a line. Having more than one particle, we could now add a new feature to the walk: entanglement between the particles. In particular, we considered initial states maximally entangled in the coin degrees of freedom and with opposite symmetries, and compared them to the case where the two particles were initially in a pure or mixed separable state (the particles being then independent or only classically correlated, respectively). We found that the entanglement in the coin states introduced spatial correlations between the particles, and that their average distance is larger in the “-” case than in the separable case, and is smaller in the “+” case. This could benefit algorithmic applications which require two marked sites to be reached which are known

a priori to be on the opposite or on the same sides of a line. We also found that the introduction of entanglement could increase or decrease the probability to find at least one particle on a given point of the line. This increase could allow us to reach a marked site faster than with two unentangled quantum walkers. The entanglement in the initial conditions thus appears as a resource that we can tune according to our needs to enhance a given application (algorithmic or other) based on a quantum walk.

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