Quantum walk on a line with two entangled particles

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(Received 8 December 2005; published 3 October 2006)

We introduce the concept of a quantum walk with two particles and study it for the case of a discrete time walk on a line. A quantum walk with more than one particle may contain entanglement, thus offering a resource unavailable in the classical scenario and which can present interesting modifications on quantum walks with single particles. In this work, we show both numerically and analytically 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, the probability to find at least one particle in a certain position after N steps of the walk, as well as the average distance and the squared distance between the two particles, can be larger or smaller than the case of two unentangled particles, depending on the initial conditions we choose. This resource can then be tuned according to our needs to modify the features of a quantum walk. Experimental implementations are briefly discussed.

DOI: 10.1103/PhysRevA.74.042304 PACS number(s): 03.67.Mn, 03.65.−w, 05.30.−d, 05.40.Fb

Quantum walks, the quantum version of random walks, were first introduced in 1993 [1] and have since then been a topic of research within the context of quantum information and computation (for an introduction, see [2]). Given the superposition principle of quantum mechanics, quantum walks allow for coherent superpositions of classical random walks and, due to interference effects, can exhibit different features and offer advantages when compared to the classical case. In particular, for a quantum walk on a line, the variance after N steps is proportional to N^2, rather than N as in the classical case (see Fig. 1). Recently, several quantum algorithms with optimal efficiency were proposed based on quantum walks [3], and it was even shown that a continuous-time quantum walk on a specific graph can be used for exponential algorithmic speedup [4].

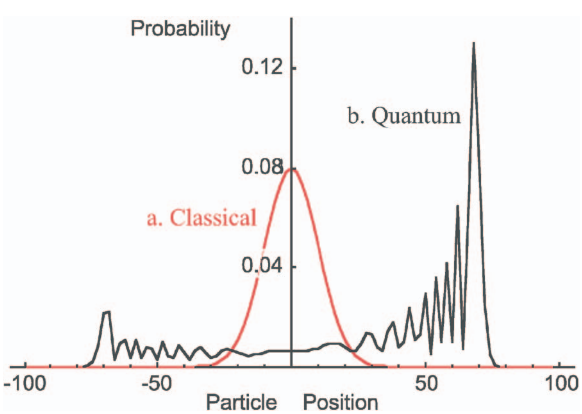

FIG. 1. (Color online) Probability distribution for a classical random walk (a) on a line after $N=100$ steps, as well as for a quantum walk (b) with initial state $|0\rangle \otimes |\uparrow\rangle$ and a Hadamard coin.

All studies on quantum walks so far have, however, been based on a single walker. In this article we study a discrete-time quantum walk on a line with two particles. Classically, random walks with K particles are equivalent to K independent single-particle random walks. In the quantum case, though, a walk with K particles may contain entanglement, thus offering a resource unavailable in the classical scenario which can introduce interesting features. Moreover, in the case of identical particles we have to take into account the effects of quantum statistics, giving an additional feature to quantum walks that can also be exploited. In this work we explicitly show that a quantum walk with two particles can indeed be tuned to behave very differently from two independent single-particle quantum walks.

Let us start by introducing the discrete-time quantum walk on a line for a single particle. The relevant degrees of freedom are the particle's position i (with $i \in \mathbb{Z}$) on the line, as well as its *coin* state. The total Hilbert space is given by $\mathcal{H} \equiv \mathcal{H}_P \otimes \mathcal{H}_C$, where $\mathcal{H}_P$ is spanned by the orthonormal vectors $\{|i\rangle\}$ representing the position of the particle and $\mathcal{H}_C$ is the two-dimensional coin space spanned by two orthonormal vectors which we denote as $|\uparrow\rangle$ and $|\downarrow\rangle$.

Each step of the quantum walk is given by two subsequent operations: the *coin operation* and the *shift-position operation*. The coin operation, given by $\hat{U}_C \in \mathrm{SU}(2)$ and acting only on $\mathcal{H}_C$, is the quantum equivalent of randomly choosing which way the particle will move (like tossing a coin in the classical case). The nonclassical character of the quantum walk is precisely here, as this operation allows for superpositions of different alternatives, leading to different moves. Then, the shift-position operation $\hat{S}$ moves the particle according to the coin state, transferring this way the quantum superposition to the total state in $\mathcal{H}$. The evolution of the system at each step of the walk can then be described by the total unitary operator

$$\hat{U} \equiv \hat{S}(\hat{I}_P \otimes \hat{U}_C), \tag{1}$$

where $\hat{I}_P$ is the identity operator on $\mathcal{H}_P$. Note that if a measurement is performed after each step, we will revert to the classical random walk.

In this article we choose to study a quantum walk with a *Hadamard coin*—i.e., where $\hat{U}_C$ is the Hadarmard operator $\hat{H}$:

$$\hat{H} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}. \tag{2}$$

Note that this represents a *balanced coin*; i.e., there is a 50-50 chance for each alternative. The shift-position operator is given by

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

Therefore, if the initial state of our particle is, for instance, $|0\rangle \otimes |\uparrow\rangle$, the first step of the quantum walk will be as follows:

$$|0\rangle \otimes |\uparrow\rangle \xrightarrow{\hat{H}} |0\rangle \otimes \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \xrightarrow{\hat{S}} \frac{1}{\sqrt{2}}(|1\rangle \otimes |\uparrow\rangle + |-1\rangle \otimes |\downarrow\rangle). \tag{4}$$

We see that there is a probability of 1/2 to find the particle in position 1, as well as to find it in position 2, just like in the classical case. Yet, if we let this quantum walk evolve for three or more steps before we perform a position measurement, we will find a very different probability distribution for the position of the particle when compared to the classical random walk, as can be seen in Fig. 1 for $N=100$ steps.

Let us consider the previous quantum walk, but now with two noninteracting particles on a line (not necessarily the same). If the particles are distinguishable and in a pure separable state, the position measurement of one particle will not change the probability distribution of the other; they are completely uncorrelated. On the other hand, if the particles are entangled, a new resource with no classical equivalent will be at our disposal.

This is a specific instance of the well-known interference phenomenon in quantum mechanics, applied to the case of a composite system. In particular, let us have a composite system consisting of two particles, labeled 1 and 2, prepared in a pure separable state,

$$|\psi^S\rangle_{12} = |\alpha\rangle_1|\beta\rangle_2, \tag{5}$$

and a general separable two-particle observable

$$\hat{A}_{12} = \hat{A}_1 \otimes \hat{A}_2. \tag{6}$$

Then, the expectation value of the observable $\hat{A}_{12}$ for a system in a state $|\psi^S\rangle_{12}$ is the simple product of the two subsystem expectation values:

$$\langle\psi^S|\hat{A}_{12}|\psi^S\rangle_{12} = \langle\alpha|\hat{A}_1|\alpha\rangle_1\langle\beta|\hat{A}_2|\beta\rangle_2. \tag{7}$$

On the other hand, if the composite system is in a general entangled state

$$|\chi^E\rangle_{12} = a|\psi^S\rangle_{12} + b|\varphi^S\rangle_{12}, \tag{8}$$

where $|a|^2+|b|^2=1$ and $|\varphi^S\rangle_{12}=|\beta\rangle_1|\alpha\rangle_2$ (with $|\alpha\rangle \neq e^{i\theta}|\beta\rangle$), then the expectation value of the observable $\hat{A}_{12}$ is given by

$$\begin{aligned}\langle\chi^E|\hat{A}_{12}|\chi^E\rangle_{12} = {} & |a|^2\langle\alpha|\hat{A}_1|\alpha\rangle_1\langle\beta|\hat{A}_2|\beta\rangle_2 \\ & + |b|^2\langle\beta|\hat{A}_1|\beta\rangle_1\langle\alpha|\hat{A}_2|\alpha\rangle_2 \\ & + a^*b\langle\alpha|\hat{A}_1|\beta\rangle_1\langle\beta|\hat{A}_2|\alpha\rangle_2 \\ & + ab^*\langle\beta|\hat{A}_1|\alpha\rangle_1\langle\alpha|\hat{A}_2|\beta\rangle_2.\end{aligned} \tag{9}$$

Note that the first two terms on the right-hand side of the above equation represent the weighted sum of the expectation values for the states $|\psi^S\rangle_{12}$ and $|\varphi^S\rangle_{12}$, with the weights $|a|^2$ and $|b|^2$, respectively. In other words, the first two terms represent the expectation value of the observable $\hat{A}_{12}$ for a mixed separable state:

$$\hat{\rho}^S_{12} = |a|^2|\psi^S\rangle\langle\psi^S|_{12} + |b|^2|\varphi^S\rangle\langle\varphi^S|_{12}. \tag{10}$$

The last two terms in Eq. (9) are purely quantum and represent the interference between the two states $|\psi^S\rangle_{12}$ and $|\varphi^S\rangle_{12}$, superposed in the state $|\chi\rangle_{12}$. Note that to obtain this purely quantum phenomenon, we need only an entangled state, even if the observable $\hat{A}_{12}=\hat{A}_1\otimes\hat{A}_2$ is separable.

Returning to the case of two walkers on a line, the joint Hilbert space of our composite system is given by

$$\mathcal{H}_{12} \equiv \mathcal{H}_1 \otimes \mathcal{H}_2 \equiv (\mathcal{H}_{P,1} \otimes \mathcal{H}_{C,1}) \otimes (\mathcal{H}_{P,2} \otimes \mathcal{H}_{C,2}), \tag{11}$$

where $\mathcal{H}_1$ and $\mathcal{H}_2$ represent the Hilbert spaces of particles 1 and 2, respectively. Since the relevant degrees of freedom in our problem are the same for both particles, we have that both $\mathcal{H}_1$ and $\mathcal{H}_2$ are isomorphic to $\mathcal{H}$ defined earlier for the one-particle case. Note also that in the case of identical particles we have to restrict $\mathcal{H}_{12}$ to its symmetrical and antisymmetrical subspaces for bosons and fermions, respectively.

Let us first consider the particular case where both particles start the quantum walk in the same position, 0, but with different coin states $|\downarrow\rangle$ and $|\uparrow\rangle$. In the case where the particles are in a pure separable state, our system's initial state will be given by

$$|\psi^S_0\rangle_{12} = |0,\downarrow\rangle_1|0,\uparrow\rangle_2. \tag{12}$$

We can also consider an initial pure state entangled in the coin degrees of freedom. In particular, we will consider the following two maximally entangled states:

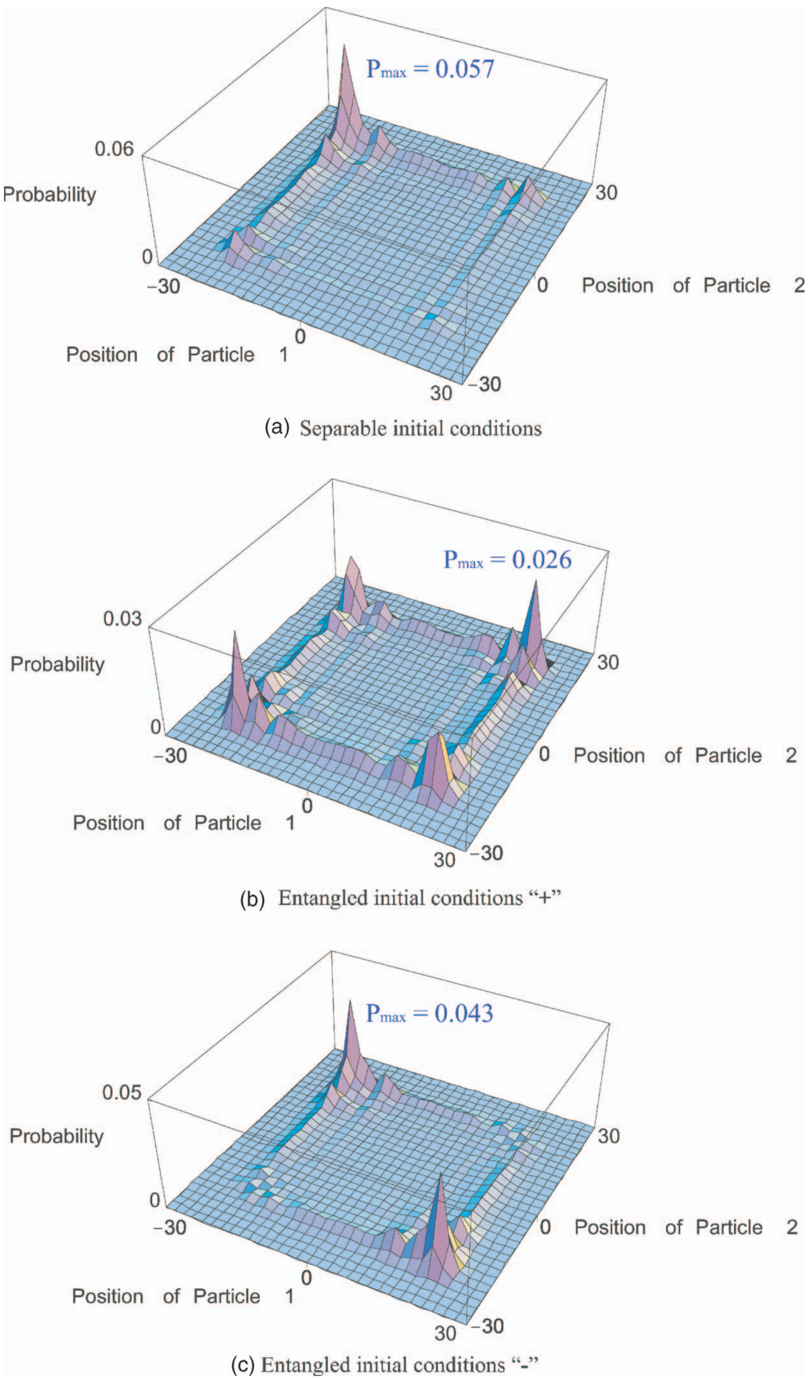

FIG. 2. (Color online) Two-particle probability distributions after $N=30$ steps for different initial conditions: (a) separable state $|\psi_0^S\rangle_{12}$, (b) $|\psi_0^+\rangle_{12}$ state, and (c) $|\psi_0^-\rangle_{12}$ state. Note the different vertical ranges.

$$|\psi_0^{\pm}\rangle_{12} = \frac{1}{\sqrt{2}}(|0,\downarrow\rangle_1|0,\uparrow\rangle_2 \pm |0,\uparrow\rangle_1|0,\downarrow\rangle_2), \qquad (13)$$

differing only by a relative phase. Note that if we were considering identical particles on the same point, our system would have to be described by these states for bosons and fermions, respectively.

Each step of this two-particle quantum walk will be given by

$$\hat{U}_{12} = \hat{U} \otimes \hat{U}, \qquad (14)$$

where $\hat{U}$ is given by Eq. (1) and is the same for both particles. After N steps, the state of the system will be, in the case of the initial conditions (12)

$$|\psi_N^S\rangle_{12} = \hat{U}_{12}^N|\psi_0^S\rangle_{12} = \hat{U}^N|0,\downarrow\rangle_1 \hat{U}^N|0,\uparrow\rangle_2. \qquad (15)$$

Figure 2(a) shows the joint probability distribution $P_{12}^S(i,j;N)$ for finding particle 1 in position i and particle 2 in position j for $N=30$ steps. Note that, since the particles are uncorrelated, $P_{12}^S(i,j;N)$ is simply the product of the two independent one-particle distributions:

$$P_{12}^S(i,j;N) = P_1^S(i;N) \times P_2^S(j;N), \tag{16}$$

where $P_1^S(i;N)$ is the probability distribution for finding particle 1 in position i after N steps and similarly for $P_2^S(j;N)$ and particle 2. This can also be observed in Fig. 2(a), which is clearly the product of two independent single-particle distributions, one biased to the left for particle 1 and the other to the right for particle 2, accordingly with the initial conditions given by Eq. (12).

In the case of entangled particles, the state of the system after N steps will be

$$|\psi_N^\pm\rangle_{12} = \hat{U}_{12}^N|\psi_0^\pm\rangle_{12} = \frac{1}{\sqrt{2}}(\hat{U}^N|0,\downarrow\rangle_1\hat{U}^N|0,\uparrow\rangle_2 \pm \hat{U}^N|0,\uparrow\rangle_1\hat{U}^N|0,\downarrow\rangle_2). \tag{17}$$

The probability distribution for finding particle 1 in position i and particle 2 in position j in the "+" case, $P_{12}^+(i,j;N)$, is represented in Fig. 2(b), for $N=30$. Similarly, Fig. 2(c) shows the distribution $P_{12}^-(i,j;N)$ of the "−" case, again for $N=30$. The effects of the entanglement are striking when comparing the three distributions in Fig. 2. In particular, we see that these effects significantly increase the probability of the particles reaching certain configurations on the line, which otherwise would be very unlikely to be occupied. In all cases, the maxima of the distributions occur around positions $\pm N/\sqrt{2} \approx \pm 20$. In the "+" case it is most likely to find both particles together, whereas for "−" the former situation is impossible and the particles will tend to finish as distant as possible from one another.

Let us now consider the individual particles in the entangled system. For instance, the state of the first particle can be described by the reduced density operator $\hat{\rho}_1(N) \equiv Tr_2(|\psi_N^\pm\rangle_{12\ 12}\langle\psi_N^\pm|)$, which consists of an equal mixture of the one-particle states $\hat{U}^N|0,\downarrow\rangle$ and $\hat{U}^N|0,\uparrow\rangle$. Thus, the probability to find particle 1 in position i after N steps is given by the following marginal probability distribution:

$$P_1^\pm(i;N) = \frac{1}{2}[P_\downarrow(i;N) + P_\uparrow(i;N)], \tag{18}$$

where $P_\downarrow(i;N)$ is the probability distribution for finding the particle in state $\hat{U}^N|0,\downarrow\rangle$ in position i after N steps and similarly for $P_\uparrow(i;N)$ and a particle in state $\hat{U}^N|0,\uparrow\rangle$. The results for particle 2 are analogous: in particular, $P_2^\pm(i;N)$ is also given by Eq. (18). Note that in the case of initial conditions (12) we have the marginal probabilities $P_1^S(i;N)=P_\downarrow(i;N)$ and $P_2^S(i;N)=P_\uparrow(i;N)$. But now, contrary to the separable case, the joint probability $P_{12}^\pm(i,j;N)$ is no longer the simple product of the two one-particle probabilities. In fact, it is not even a weighted sum of productlike terms as it contains the interference part analogous to the one from Eq. (9), giving information about the nontrivial *quantum* correlations between the outcomes of the position measurement performed on each particle. From Eq. (17), it follows that the probability $P_{12}^\pm(i,j;N)$ is given by

TABLE I. Average product $\langle\hat{x}_1\hat{x}_2\rangle^{S,\pm}$ after N steps, for the initial conditions $|\psi_0^-\rangle_{12}$, $|\psi_0^S\rangle_{12}$, and $|\psi_0^+\rangle_{12}$.

	Expectation value $\langle\hat{x}_1\hat{x}_2\rangle^{S,\pm}$ after N steps					
N	10	20	30	40	60	100
$\|\psi_0^-\rangle_{12}$	−16.8	−69.8	−153.5	−276.2	−619.7	−1718.3
$\|\psi_0^S\rangle_{12}$	−6.0	−31.3	−69.9	−130.5	−298.3	−839.6
$\|\psi_0^+\rangle_{12}$	4.8	7.3	13.7	15.1	23.1	39.1

$$P_{12}^\pm(i,j;N) = \frac{1}{2}\{P_{\downarrow\uparrow}(i,j;N) + P_{\uparrow\downarrow}(i,j;N) \pm [\mathcal{I}_{\downarrow\uparrow}(i;N)\mathcal{I}_{\uparrow\downarrow}(j;N) + \mathcal{I}_{\uparrow\downarrow}(i;N)\mathcal{I}_{\downarrow\uparrow}(j;N)]\}, \tag{19}$$

where $P_{\downarrow\uparrow}(i,j;N)=P_\downarrow(i;N)P_\uparrow(j;N)$ and $\mathcal{I}_{\downarrow\uparrow}(i;N) = \langle 0,\downarrow|(\hat{U}^\dagger)^N|i\rangle\langle i|\hat{U}^N|0,\uparrow\rangle$ [and analogously for $P_{\uparrow\downarrow}(i,j;N)$ and $\mathcal{I}_{\downarrow\uparrow}(i;N)$]. Therefore, to investigate more quantitatively the difference between quantum walks with two distinguishable particles in a pure separable state and two particles entangled in their coin degree of freedom, we must look at joint (two-particle) rather than individual properties.

First, let us consider a simple product $\hat{x}_1\hat{x}_2$ between the subsystem position operators $\hat{x}_1$ and $\hat{x}_2$ for particles 1 and 2, respectively (note that for simplicity, we have omitted to write the dependence on the number of steps, N). The expectation values $\langle\hat{x}_1\hat{x}_2\rangle^{S,\pm}$ for the three initial states $|\psi_0^S\rangle_{12}$ and $|\psi_0^\pm\rangle_{12}$ are presented in Table I for different N. We observe that the three cases are "equidistant" in the sense that, for each N, the following relation holds:

$$\langle\hat{x}_1\hat{x}_2\rangle^- - \langle\hat{x}_1\hat{x}_2\rangle^S = \langle\hat{x}_1\hat{x}_2\rangle^S - \langle\hat{x}_1\hat{x}_2\rangle^+. \tag{20}$$

In order to study the above quantity analytically, let us write the definition of the expectation value $\langle\hat{x}_1\hat{x}_2\rangle \equiv \sum_{i,j=-N}^N ijP_{12}(i,j;N)$. Using Eqs. (16) and (19) for the joint probability distributions $P_{12}^S(i,j;N)$ and $P_{12}^\pm(i,j;N)$, respectively, we get the following expression:

$$\langle\hat{x}_1\hat{x}_2\rangle^\pm = \langle\hat{x}_1\hat{x}_2\rangle^S \pm \frac{1}{2}\sum_{i,j=-N}^N ij[\mathcal{I}_{\downarrow\uparrow}(i;N)\mathcal{I}_{\uparrow\downarrow}(j;N) + \mathcal{I}_{\uparrow\downarrow}(i;N)\mathcal{I}_{\downarrow\uparrow}(j;N)]. \tag{21}$$

We immediately see that the relation (20) is indeed satisfied for every N. If by $\langle\hat{x}_\downarrow\rangle$ we denote the average position for the one-particle probability distribution $P_\downarrow(i;N)$ and analogously for $\langle\hat{x}_\uparrow\rangle$, we also have that $\langle\hat{x}_1\hat{x}_2\rangle^S=\langle\hat{x}_\downarrow\rangle\langle\hat{x}_\uparrow\rangle=-\langle\hat{x}_\downarrow\rangle^2$ as $P_\downarrow(i;N)=P_\uparrow(-i;N)$. Using the obvious relation $\mathcal{I}_{\downarrow\uparrow}(i;N) = \mathcal{I}_{\uparrow\downarrow}^*(i;N)$, we can further simplify expression (21) by writing

$$\langle\hat{x}_1\hat{x}_2\rangle^\pm = -\langle\hat{x}_\downarrow\rangle^2 \pm \|I_{\downarrow\uparrow}\|^2, \tag{22}$$

with $I_{\downarrow\uparrow}=\sum_{i=-N}^N i\mathcal{I}_{\downarrow\uparrow}(i;N)$.

To analyze the asymptotic behavior of $\langle\hat{x}_1\hat{x}_2\rangle$ for large N, we use the technique developed in [6] based on Fourier analysis (for an alternative treatment, see [7]). There, it was shown that for every initial coin state, the expectation value of the position operator in a one-particle quantum walk on a line has a linear drift $\langle \hat{x} \rangle \propto N$, for N large enough. Following [6], we can express $I_{\downarrow\uparrow}$ as

$$I_{\downarrow\uparrow} = -\frac{1}{2\pi}\sum_{j=1}^{N}\int_{-\pi}^{\pi} dk \langle \downarrow | (\hat{H}_k^{\dagger})^j \hat{Z} (\hat{H}_k)^j | \uparrow \rangle, \tag{23}$$

with $\hat{Z} \equiv \hat{I}_C - 2|\downarrow\rangle\langle\downarrow|$ and

$$\hat{H}_k = \frac{1}{\sqrt{2}} \begin{bmatrix} e^{-ik} & e^{-ik} \\ e^{ik} & -e^{ik} \end{bmatrix}.$$

Let $|\phi_{kl}\rangle$ be eigenvectors for the operators $\hat{H}_k$, with eigenvalues $e^{\theta_{kl}}$, and let $|\uparrow\rangle = \Sigma_{l=1}^2 u_{kl}|\phi_{kl}\rangle$ and $|\downarrow\rangle = \Sigma_{l=1}^2 d_{kl}|\phi_{kl}\rangle$. Then, Eq. (23) can be rewritten in the following way ($\hat{P}_\downarrow \equiv |\downarrow\rangle\langle\downarrow|$):

$$I_{\downarrow\uparrow} = -N + \frac{1}{\pi}\int_{-\pi}^{\pi} dk \sum_{l,l'=1}^{2} u_{kl}^* d_{kl'} \langle \phi_{kl} | \hat{P}_\downarrow | \phi_{kl'} \rangle \sum_{j=1}^{N} e^{i(\theta_{kl'} - \theta_{kl}) j}. \tag{24}$$

Since for $l \neq l'$ the terms in the above equation are oscillatory, for large N they will average to zero, thus yielding the linear asymptotic behavior of $I_{\downarrow\uparrow}$ with respect to the number of steps:

$$I_{\downarrow\uparrow} = E_1 N, \tag{25}$$

where $E_1 = -1 + (1\pi)\int_{-\pi}^{\pi} dk \Sigma_l u_{kl}^* d_{kl} \langle \phi_{kl} | \hat{P}_\downarrow | \phi_{kl} \rangle$. Combining the above result with Eq. (22) and the asymptotic behavior $\langle \hat{x} \rangle \propto N$, we conclude that in general $\langle \hat{x}_1 \hat{x}_2 \rangle$, as well as the "distances" given by Eq. (20), should scale quadratically with the number of steps N. Looking at the numerical results presented in Table I, we see that for $|\psi_0^-\rangle_{12}$ and $|\psi_0^S\rangle_{12}$ initial states we indeed have that $\langle \hat{x}_1 \hat{x}_2 \rangle^{S,-} \propto N^2$, while for the $|\psi_0^+\rangle_{12}$ initial state we have that $\langle \hat{x}_1 \hat{x}_2 \rangle^+ \propto N$. In other words, the quadratic parts of $\langle \hat{x}_\downarrow \rangle^2$ and $\|I_{\downarrow\uparrow}\|^2$ cancel out each other for the case of $|\psi_0^+\rangle_{12}$ initial state. We performed numerical simulations up to $N=8000$ steps, and they confirmed the behavior presented in Table I.

Note that these effects require the presence of entanglement in the initial conditions. For instance, $P_{12}^-(i,j;N)$ can never be obtained from *separable* initial states of the coins. Suppose that, given a general separable (possibly mixed) initial state of the coins, one has to achieve in N steps as negative a value of $\langle \hat{x}_1 \hat{x}_2 \rangle$ as possible by starting the walkers in the position state $|0\rangle_1|0\rangle_2$. For such states, $\langle \hat{x}_1 \hat{x}_2 \rangle$ is simply a weighted average of $\langle \hat{x}_1 \rangle \langle \hat{x}_2 \rangle$ over several pure product states. Now, it is well known that for single-particle walks with the Hadamard coin, $|0,\uparrow\rangle_i$ and $|0,\downarrow\rangle_i$ give the most positive and the most negative values of $\langle \hat{x}_i \rangle$, respectively [2] (they give the most asymmetric distributions for the walkers' position). Thus, for two-particle walks, a set of separable states for most negative $\langle \hat{x}_1 \hat{x}_2 \rangle$ are mixed states of the form $\hat{\rho}^A = \mathcal{P}|\psi_0^S\rangle\langle\psi_0^S| + (1-\mathcal{P})|\psi_0^{S'}\rangle\langle\psi_0^{S'}|$, where $|\psi_0^{S'}\rangle_{12} = |0,\uparrow\rangle_1|0,\downarrow\rangle_2$ and $\mathcal{P}$ is any probability. Mixing *any* state $|0,\nearrow\rangle_1|0,\searrow\rangle_2$ with $\hat{\rho}^A$, where $|\nearrow\rangle$ and $|\searrow\rangle$ are arbitrary states of the coins (not necessarily orthogonal to each other), even with an arbitrarily small probability, will make $\langle \hat{x}_1 \hat{x}_2 \rangle$ more positive or keep it unchanged at best. However, from Eqs. (21) and (22), we see that $\langle \hat{x}_1 \hat{x}_2 \rangle^- < \langle \hat{x}_1 \hat{x}_2 \rangle^S$ for every N. Thus, the expectation value $\langle \hat{x}_1 \hat{x}_2 \rangle$ of $P_{12}^-(i,j;N)$ is always more negative than that obtained with *any* separable state. Therefore, $P_{12}^-(i,j;N)$ cannot be reproduced with a walk starting in $|0\rangle_1|0\rangle_2$ that has a separable initial state of the coins.

For a general pure entangled coin state we can write the overall initial state as follows:

$$|\psi_0\rangle_{12} = |00\rangle_{12} \otimes (\alpha|\uparrow\uparrow\rangle_{12} + \beta|\uparrow\downarrow\rangle_{12} + \gamma|\downarrow\uparrow\rangle_{12} + \delta|\downarrow\downarrow\rangle_{12}), \tag{26}$$

with $|\alpha|^2 + |\beta|^2 + |\gamma|^2 + |\delta|^2 = 1$. From the above discussion, it follows that the expectation value of operator $\hat{x}_1 \hat{x}_2$ can be written in the following form:

$$\begin{aligned} \langle \hat{x}_1 \hat{x}_2 \rangle &= (|\alpha|^2 + |\delta|^2 - |\beta|^2 - |\gamma|^2)\langle \hat{x}_\downarrow \rangle^2 \\ &\quad + 2\langle \hat{x}_\downarrow \rangle \mathrm{Re}[(-\alpha\beta^* - \alpha\gamma^* + \gamma\delta^* + \beta\delta^*) I_{\downarrow\uparrow}] \\ &\quad + 2\,\mathrm{Re}[(\alpha\delta^* + \beta\gamma^*) I_{\downarrow\uparrow}^2], \end{aligned} \tag{27}$$

where $\mathrm{Re}[z]$ is real part of a complex number z. The initial entangled states $|\psi_0^\pm\rangle_{12}$ discussed above correspond to the choice of coefficients $\alpha = \delta = 0$ and $\gamma = \pm\beta = 1/\sqrt{2}$. We see that by taking as initial coin states the other two Bell states (corresponding to the choice of $\beta = \gamma = 0$ and $\delta = \pm\alpha = 1/\sqrt{2}$)

$$|\phi_0^\pm\rangle_{12} = \frac{1}{\sqrt{2}}(|0,\downarrow\rangle_1|0,\downarrow\rangle_2 \pm |0,\uparrow\rangle_1|0,\uparrow\rangle_2), \tag{28}$$

we obtain analogous results: $|\phi_0^\pm\rangle_{12}$ are "equidistant" from the separable initial states $|0,\downarrow\rangle_1|0,\downarrow\rangle_2$ and $|0,\uparrow\rangle_1|0,\uparrow\rangle_2$ [in the sense of Eq. (20)], with $|\phi_0^+\rangle_{12}$ achieving the maximal positive value for $\langle \hat{x}_1 \hat{x}_2 \rangle$, which has the same absolute value as the one obtained for the $|\psi_0^-\rangle_{12}$ initial state.

Finally, we note that the above results for $\langle \hat{x}_1 \hat{x}_2 \rangle$ [Eq. (22) and Table I], together with the results for $\langle \hat{x} \rangle$ of a single-particle quantum walk on a line (see [6]), offer us an explicit form for the correlation function $C_{12} \equiv \langle \hat{x}_1 \hat{x}_2 \rangle - \langle \hat{x}_1 \rangle \langle \hat{x}_2 \rangle$.

The second quantity we choose to study is the squared distance between the two particles, defined as

$$\langle \hat{\Delta}_{12}^2 \rangle \equiv \langle (\hat{x}_1 - \hat{x}_2)^2 \rangle. \tag{29}$$

Again, it represents a joint property. The expectation values $\langle \hat{\Delta}_{12}^2 \rangle^{S,\pm}$ for the three initial states $|\psi_0^S\rangle_{12}$ and $|\psi_0^\pm\rangle_{12}$ are presented in Table II for different N. We see that in the "−" case the particles tend, on average, to end the quantum walk more distant from each other, whereas in the "+" case they tend to stay closer and somewhere in between in the separable case. In fact, for fixed N, we have a relation analogous to Eq. (20):

$$\langle \hat{\Delta}_{12}^2 \rangle^- - \langle \hat{\Delta}_{12}^2 \rangle^S = \langle \hat{\Delta}_{12}^2 \rangle^S - \langle \hat{\Delta}_{12}^2 \rangle^+. \tag{30}$$

This can be shown to be a general property if we express $\langle \hat{\Delta}_{12}^2 \rangle$ in the following way:

TABLE II. Average squared distance $\langle\hat{\Delta}_{12}^2\rangle^{S,\pm}$ after N steps, for the initial conditions $|\psi_0^-\rangle_{12}$, $|\psi_0^S\rangle_{12}$, and $|\psi_0^+\rangle_{12}$.

	Expectation value $\langle\hat{\Delta}_{12}^2\rangle^{S,\pm}$ after N steps					
N	10	20	30	40	60	100
$\|\psi_0^-\rangle_{12}$	93.6	374.8	835.4	1490.5	3349.1	9295.4
$\|\psi_0^S\rangle_{12}$	71.9	297.7	668.2	1199.2	2706.4	7538.0
$\|\psi_0^+\rangle_{12}$	50.3	220.6	501.1	907.9	2063.6	5780.6

$$\langle\hat{\Delta}_{12}^2\rangle = \langle\hat{x}_1^2\rangle + \langle\hat{x}_2^2\rangle - 2\langle\hat{x}_1\hat{x}_2\rangle. \tag{31}$$

Using the previous discussion for $\langle\hat{x}_1\hat{x}_2\rangle$, we see that the relation (30) is just a consequence of the result (22), as in all three cases we have that $\langle\hat{x}_1^2\rangle=\langle\hat{x}_2^2\rangle=\langle\hat{x}_\downarrow^2\rangle$, with $\langle\hat{x}_\downarrow^2\rangle$ being the mean-squared position for the probability distribution $P_\downarrow(i;N)$. In the case of a general initial coin state (26), the analytical result for $\langle\hat{\Delta}_{12}^2\rangle$ is obtained using Eq. (27) together with

$$\langle\hat{x}_1^2\rangle = \langle\hat{x}_\downarrow^2\rangle + 2\,\mathrm{Re}[(\alpha\beta^* + \gamma\delta^*)K_{\downarrow\uparrow}], \tag{32}$$

where $K_{\downarrow\uparrow}=\sum_{i=-N}^{N} i^2\langle 0,\downarrow|(\hat{U}^\dagger)^N|i\rangle\langle i|\hat{U}^N|0,\uparrow\rangle$ (and the analogous expression for $\langle\hat{x}_2^2\rangle$). Then, further analysis of the quantity $K_{\downarrow\uparrow}$ can be carried out in a similar fashion to the one done for $I_{\downarrow\uparrow}$ (see also [6]). The main conclusion of this analysis is that, asymptotically, $\langle\hat{\Delta}_{12}^2\rangle$ scales quadratically with the number of steps, N, which is confirmed by numerics as well; see Table II (again, we performed numerical simulations up to $N=8000$ steps, confirming the results presented in Table II).

If instead of the squared distance we choose the linear distance itself, given by $\langle\hat{\Delta}_{12}\rangle=\langle|\hat{x}_1-\hat{x}_2|\rangle$, we obtain the results presented in Table III. Again, we observe behavior analogous to that given by Eqs. (20) and (30). Furthermore, we see that the distance scales linearly with N.

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

$$\begin{aligned}\mathcal{P}^{S,\pm}(i;N) &= \sum_{j=-N}^{N}[P_{12}^{S,\pm}(i,j;N) + P_{12}^{S,\pm}(j,i;N)] - P_{12}^{S,\pm}(i,i;N)\\ &= [P_1^{S,\pm}(i;N) + P_2^{S,\pm}(i;N)] - P_{12}^{S,\pm}(i,i;N)\\ &= [P_\downarrow(i;N) + P_\uparrow(i;N)] - P_{12}^{S,\pm}(i,i;N).\end{aligned} \tag{33}$$

TABLE III. Average distance $\langle\hat{\Delta}_{12}\rangle^{S,\pm}$ after N steps, for the initial conditions $|\psi_0^-\rangle_{12}$, $|\psi_0^S\rangle_{12}$, and $|\psi_0^+\rangle_{12}$.

	Expectation value $\langle\hat{\Delta}_{12}\rangle^{S,\pm}$ after N steps					
N	10	20	30	40	60	100
$\|\psi_0^-\rangle_{12}$	8.8	17.5	26.0	34.9	52.2	87.0
$\|\psi_0^S\rangle_{12}$	7.1	14.7	21.9	29.5	44.3	73.9
$\|\psi_0^+\rangle_{12}$	5.5	11.9	17.8	24.1	36.3	60.8

From Eqs. (16) and (19), it follows that $P_{12}^{\pm}(i,i;N) = P_{12}^{S}(i,i;N) \pm \|\mathcal{I}_{\downarrow\uparrow}(i,i;N)\|^2$, so that

$$\mathcal{P}^-(i;N) > \mathcal{P}^S(i;N) > \mathcal{P}^+(i;N). \tag{34}$$

We see that, by introducing entanglement in the initial conditions of our two-particle quantum walk, the probability of finding at least one particle in a particular position on the line can actually be better or worse 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 Eq. (13) are maximally entangled, but rather on their symmetry-relative phase.

This work allows for generalizations in a number of ways. First, one could consider periodic or other boundary conditions on the line or more general graphs [5]. Note that the positions on the line of our two particles could also be interpreted as the position of a single particle doing the quantum walk on a regular two-dimensional lattice. More general coins could also be considered [8–10], including entangling and nonbalanced coins, as well as different initial states. One could also augment the number of particles and study these quantum walks in continuous time or in their asymptotic limit. Furthermore, also very interesting and promising is to investigate the use of multiparticle quantum walks in solving mathematical or practical problems that could be encoded as a quantum walk, such as the estimation of the volume of a convex body [11] or the connectivity in a P2P network [12].

Finally, we present some brief comments about implementations of our two-particle quantum walk on a line. The methods recently proposed for the single-particle case using cavity QED [13], optical lattices [14], or ion traps [15] could be adapted to our two-particle case. For instance, in the latter we could encode the coin states in the electronic levels of two ions and the position in their *center-of-mass* 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 [16]. 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 [8,17]. Note that this could be implemented with other particles as well—e.g., electrons—using a device equivalent to a beam splitter [18]. Also very interesting, regardless of any particular method or technology, is the possibility of using two indistinguishable particles on the same line to implement our quantum walk. Say we encode the coin degrees of freedom in the polarization of two photons or in the spin of two electrons: if the two particles start in the same position 0, then they will be forced to be in the states given by Eq. (13) ("+" for bosons and "−" for fermions). Although the particles will initially be only entangled in the mathematical sense (as they cannot be addressed to extract quantum correlations), this is a perfectly valid way of preparing the $|\psi_0^+\rangle_{12}$ and $|\psi_0^-\rangle_{12}$ initial states for our quantum walk, saving us the trouble of generating entangled pairs. Thus, the indistinguishability of identical particles appears as a resource, much in the same manner as it can play an useful role in quantum-information processing [19]. Here, in particular, the indistinguishability of identical particles offers a way to simplify the preparation of the initial states for a two-particle quantum walk on a line.

The fermionic and bosonic nature of identical particles in quantum mechanics can also be used to *explain* the behavior we have obtained above for our quantum walk with two entangled particles on the same line. Although we consider our particles to be distinguishable, the specific entangled states $|\psi_0^{\mp}\rangle_{12}$ they start in are either symmetric or antisymmetric with respect to the exchange of the indices of the particles. Both the $\hat{H}$ and the $\hat{S}$ operations can be applied through global fields, as they act on both the coins. In other words, there is no need to distinguish the coins through their labels 1 and 2 to accomplish the quantum walk we describe, and the particles could as well have been indistinguishable. One would thus get precisely the *same* results as the "−" and "+" cases if one started with two fermions at $|0\rangle$ and two bosons at $|0\rangle$, respectively. The two cases exhibit typically fermionic and bosonic behaviors, with the two particles, respectively, avoiding each other or tending to bunch together, as imposed by the symmetrization postulate of quantum mechanics [20], during their quantum walk on the line.

In this article we introduced the concept of a quantum walk with two particles and studied it both numerically and analytically 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. For a general initial state of two particles starting both in position 0, we found analytical expressions for $\langle \hat{x}_1 \hat{x}_2 \rangle$ and the average squared distance and studied their asymptotic behavior. In particular, we considered initial states maximally entangled in the coin degrees of freedom and with opposite symmetries and compared them to a case where the two particles were initially unentangled. 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 unentangled case and is smaller in the "+" case. We justified that no separable state (pure or mixed) can ever generate the probability distribution obtained for the "−" case, which shows that quantum walks with two entangled particles can offer features that are unattainable in the separable case. If it was given *a priori* that the two walkers need to hit (meaning "reach with a significant probability") two sites along the line which are anticorrelated (i.e., $x_1 = -x_2$) with a certain probability (but not with unit probability, so that one still needs to search for both the sites), then a two-particle walk starting in the "−" state could do better than any separable state. The entanglement in the initial conditions thus appears as a resource that we can tune according to our needs to enhance a given application based on a quantum walk. The possibility of also playing a role in the development of quantum algorithms seems worthwhile exploring.

The authors would like to thank K. Banaszek, E. Kashefi, and T. Schaetz for precious discussions, as well as P. Mateus, A. Andrić, and R. Chadha for their help in numerical simulations. Y.O. and N.P. gratefully acknowledge support from Fundação para a Ciência e a Tecnologia (Portugal)—namely, through programs POCTI/POCI and CLC project POCI/MAT/55796/2004 QuantLog, partially funded by FEDER and the 3rd Community Support Framework of the European Social Fund. The research of Y.O. and N.P. is also developed under the scope of the cooperation agreement 24P-22335/04 between CLE-UNICAMP and CLC-UTL. Y.O. wishes to thank the Clarendon Laboratory for its hospitality. N.P. thanks the financial support of Elsag S.p.A. and of the European Commission, Contract No. IST-2001-39215 TOPQIP. L.S. gratefully acknowledges the support of the Nuffield Foundation. Finally, Y.O. and S.B. would like to acknowledge support from CRUP/BC Collaboration Grant No. B-22/05 and thank the Institute for Quantum Information at Caltech, where this work was started, for its hospitality.

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