Quantum walk on the line: Entanglement and nonlocal initial conditions

G. Abal,* R. Siri, A. Romanelli, and R. Donangelo†
Instituto de Física, Universidad de la República, C.C. 30, C.P. 11000, Montevideo, Uruguay
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The conditional shift in the evolution operator of a quantum walk generates entanglement between the coin and position degrees of freedom. This entanglement can be quantified by the von Neumman entropy of the reduced density operator (entropy of entanglement). We show analytically that for a Hadamard walk with local initial conditions the asymptotic entanglement is 0.872 for all initial coin states. When nonlocal initial conditions are considered, the asymptotic entanglement varies smoothly between almost complete entanglement and no entanglement (product state). An exact expression for the asymptotic (long-time) entanglement is obtained for initial conditions in the position subspace spanned by $|\pm 1\rangle$.

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I. INTRODUCTION

Quantum walks in several topologies [1] are being studied as potential sources for new quantum algorithms. Recently, quantum search algorithms based on different versions of the quantum walk, have been proposed [2,3]. These algorithms take advantage of quantum parallelism, but do not make use of entanglement, which has only recently begun to be addressed in the context of quantum walks. The first studies [4,5] where numerical and considered walkers driven by two coins which where maximally entangled by their initial condition. More recently, Carneiro and co-workers [6] have considered the coin-position entanglement induced by the the evolution operator. They quantified this entanglement as a function of coin bias, using the von Neumann entropy of the reduced von Neumann operator (entropy of entanglement). It was numerically established that for all coin initial states of a Hadamard walk, the entanglement has the limiting value 0.872.

In this work we use the Fourier representation of the Hadamard walk on a line to obtain this result analytically. Furthermore, using the same techniques, we may show that when nonlocal initial conditions are considered the asymptotic entanglement changes smoothly between two well defined limits, which we calculate exactly. In the long-time limit, the dependence of the entropy of entanglement on the initial conditions (which we restrict to a certain position subspace) is given.

This work is organized as follows. In Sec. II, we briefly review the discrete-time quantum walk on the line and define the entropy of entanglement. To illustrate the general method, the asymptotic value for the entanglement of a particular localized initial condition is obtained analytically. Section III is devoted to the calculation of the asymptotic entanglement induced by the evolution operator of a Hadamard walk for a particular class of nonlocal initial conditions. We show analytically that in this case, the asymptotic entanglement varies smoothly between two well defined limits. Finally, in Sec. IV we summarize our conclusions and discuss future developments.

II. DISCRETE-TIME QUANTUM WALK ON THE LINE

The discrete-time quantum walk can be thought as a quantum analog of the classical random walk where the classical coin flipping is replaced by a Hadamard operation in an abstract two-state quantum space (the coin space). A step of the quantum walker consists of a conditional traslation on the line. Of course, if the quantum coin is measured before taking a step, the classical walk is recovered [7,8]. The Hilbert space $\mathcal{H}=\mathcal{H}_P\otimes\mathcal{H}_C$, is composed of two parts: a spatial subspace $\mathcal{H}_P$ spanned by the orthonormal set $\{|x\rangle\}$ where the integers $x=0,\pm 1,\pm 2,\ldots$, are associated to discrete positions on the line and a single-qubit coin space $\mathcal{H}_C$ spanned by two orthonormal vectors denoted $\{|R\rangle,|L\rangle\}$. A generic state for the walker is

$$|\Psi\rangle=\sum_{x=-\infty}^{\infty}|x\rangle\otimes[a_x|R\rangle+b_x|L\rangle] \tag{1}$$

in terms of complex coefficients satisfying the normalization condition $\Sigma_x|a_x^2|+|b_x|^2=1$ (in what follows, the summation limits are left implicit).

A step of the walk is described by the unitary operator

$$U=S\cdot(I_P\otimes C), \tag{2}$$

where C is a suitable unitary operation in $\mathcal{H}_C$ and I_P is the identity in $\mathcal{H}_P$. A convenient choice is a Hadamard operation, $H|R\rangle=(|R\rangle+|L\rangle)/\sqrt{2}$ and $H|L\rangle=(|R\rangle-|L\rangle)/\sqrt{2}$. When $C=H$, as in this work, one refers to the process as a Hadamard walk. The shift operator

$$S=S_R\otimes|R\rangle\langle R|+S_L\otimes|L\rangle\langle L| \tag{3}$$

with $S_R=\Sigma_x|x+1\rangle\langle x|$ and $S_L=S_R^\dagger=\Sigma_x|x-1\rangle\langle x|$, conditionally shifts the position one step to the right (left) for coin state R (L). Furthermore, it generates entanglement between the coin and position degrees of freedom.

The evolution of an initial state $|\Psi(0)\rangle$ is given by

*Electronic address: abal@fing.edu.uy
†Permanent address: Instituto de Física, Universidade Federal do Rio de Janeiro, C.P. 68528, Rio de Janeiro 21941-972, Brazil

$$|\Psi(t)\rangle = U^t|\Psi(0)\rangle, \tag{4}$$

where the non-negative integer t counts the discrete time steps that have been taken. The probability distribution for finding the walker at site x at time t is $P(x;t)=|\langle x|\Psi(t)\rangle|^2 = |a_x|^2+|b_x|^2$. The variance of this distribution increases quadratically with time [9] as opposed to the classical random walk, in which the increase is only linear. This advantage in the spreading speed in the quantum case is directly related to quantum interference effects and is eventually lost in the presence of decoherence [8].

One of the early papers on quantum walks, due to Nayak and Vishwanath [10], has shown that Fourier analysis can be successfully used to obtain integral expressions for the amplitudes $a_x(t)$ and $b_x(t)$ for given initial conditions. The resulting quadratures can be evaluated in the long-time limit. The usefulness of this approach has been limited because the detailed calculations are lengthy and must be individually worked out for each initial condition. In this paper, we shall use the dual Fourier space to obtain information about the asymptotic entanglement, and so we review those results.

A. Fourier transform

The dual space $\tilde{\mathcal{H}}_k$ is spanned by the Fourier transformed kets $|k\rangle=\Sigma_x e^{ikx}|x\rangle$, where the wave number k is real and restricted to $[-\pi,\pi]$. The state vector (1) can then be written

$$|\Psi\rangle = \int_{-\pi}^{\pi} \frac{dk}{2\pi}|k\rangle \otimes [\tilde{a}_k|R\rangle + \tilde{b}_k|L\rangle], \tag{5}$$

where the k amplitudes $\tilde{a}_k=\langle k,R|\Psi\rangle$ and $\tilde{b}_k=\langle k,L|\Psi\rangle$ are related to the position amplitudes by

$$\tilde{a}_k = \sum_x e^{-ikx}a_x \text{ and } \tilde{b}_k = \sum_x e^{-ikx}b_x. \tag{6}$$

The shift operator, defined in Eq. (3), is diagonal in $\tilde{\mathcal{H}}_k$ space: $S|k,R\rangle=e^{-ik}|k,R\rangle$ and $S|k,L\rangle=e^{ik}|k,L\rangle$. A step in the evolution may be expressed through the evolution operator U_k in k space as

$$|\Phi_k(t+1)\rangle = U_k|\Phi_k(t)\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{-ik} & e^{-ik} \\ e^{ik} & -e^{ik} \end{pmatrix}|\Phi_k(t)\rangle, \tag{7}$$

where $|\Phi_k\rangle=\langle k|\Psi\rangle$ is the spinor $(\tilde{a}_k,\tilde{b}_k)^T$. This operator has eigenvectors $|\varphi_k^{(1,2)}\rangle$ given by

$$|\varphi_k^{(1)}\rangle = \alpha_k\begin{pmatrix} u_k \\ v_k \end{pmatrix}, \quad |\varphi_k^{(2)}\rangle = t a_k\begin{pmatrix} u_k \\ w_k \end{pmatrix}, \tag{8}$$

where α_k and β_k are the real, positive functions,

$$\alpha_k \equiv \frac{1}{\sqrt{2}}[1+\cos^2 k - \cos k\sqrt{1+\cos^2 k}]^{-1/2},$$

$$\beta_k \equiv \frac{1}{\sqrt{2}}[1+\cos^2 k + \cos k\sqrt{1+\cos^2 k}]^{-1/2}, \tag{9}$$

and

$$u_k \equiv e^{-ik},$$

$$v_k = \sqrt{2}e^{-i\omega_k} - e^{-ik},$$

$$w_k = -\sqrt{2}e^{i\omega_k} - e^{-ik}. \tag{10}$$

The frequency ω_k, defined by

$$\sin\omega_k \equiv \frac{\sin k}{\sqrt{2}}, \quad \omega_k \in [-\pi/2,\pi/2], \tag{11}$$

determines the eigenvalues $\pm e^{\mp i\omega_k}$ of U_k. Using the spectral decomposition for U_k, the time evolution of an initial spinor can be expressed as

$$\begin{aligned}|\Phi_k(t)\rangle &= U_k^t|\Phi_k(0)\rangle \\ &= e^{-i\omega_k t}\langle\varphi_k^{(1)}|\Phi_k(0)\rangle|\varphi_k^{(1)}\rangle + (-1)^t e^{i\omega_k t}\langle\varphi_k^{(2)}|\Phi_k(0)\rangle \\ &\quad\times|\varphi_k^{(2)}\rangle.\end{aligned} \tag{12}$$

In principle, this expression can be transformed back to position space and the probability distribution $P(x,t)$ can be obtained. This approach requires evaluation of complicated integrals which, for arbitrary times, can only be done numerically. However, in the long time limit, stationary phase methods can be used to approximate the resulting integrals for given initial conditions, an approach illustrated in Ref. [10]. In this work, we bypass these technical difficulties, because the asymptotic entanglement introduced by U_k^t, may be quantified directly from Eq. (12), without transforming back to position space.

B. Entropy of entanglement

Consider the density operator $\rho=|\Psi\rangle\langle\Psi|$. Entanglement for pure states can be quantified by the von Neumann entropy of the reduced density operator $\rho_c=\mathrm{tr}(\rho)$, where the partial trace is taken over position (or alternatively, wavenumber k). Note that, in general $\mathrm{tr}(\rho_c^2)<1$, i.e., the reduced operator ρ_c corresponds to a statistical mixture. The associated von Neumann entropy

$$S_E = -\mathrm{tr}(\rho_c \log_2 \rho_c), \tag{13}$$

also known as entropy of entanglement, quantifies the quantum correlations present in the pure state ρ [11]. It is zero for a product state and unity for a maximally entangled coin state. It is also invariant under local unitary transformations, a usual requirement for entanglement measures [12,13].

The entropy of entanglement can be obtained after diagonalization of ρ_c. This operator, which acts in $\mathcal{H}_C$, is represented by the Hermitean matrix

$$\rho_c = \begin{pmatrix} A & B \\ B^* & C \end{pmatrix}, \tag{14}$$

where

$$A \equiv \sum_x |a_x|^2 = \int_{-\pi}^{\pi} \frac{dk}{2\pi} |\tilde{a}_k|^2,$$

$$B \equiv \sum_x a_x b_x^* = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \tilde{a}_k \tilde{b}_k^*,$$

$$C \equiv \sum_x |b_x|^2 = \int_{-\pi}^{\pi} \frac{dk}{2\pi} |\tilde{b}_k|^2. \tag{15}$$

Normalization requires that $\mathrm{tr}(\rho)=1$ and $A+C=1$. The real, positive eigenvalues r_1 and r_2 of this operator are given by

$$r_{1,2} = \frac{1}{2}[1 \pm \sqrt{1+4(|B|^2 - AC)}] \tag{16}$$

and the reduced entropy can be calculated from Eq. (13) as

$$S_E = -(r_1 \log_2 r_1 + r_2 \log_2 r_2). \tag{17}$$

The entropy of entanglement has been used to quantify entanglement in the quantum walk [6]. In the particular case of a Hadamard walk, it was numerically established that the reduced entropy approaches the well-defined asymptotic value $S_E \to 0.872,\ldots$, for arbitrary initial coin states when starting from $|0\rangle$. In the rest of this work, we shall be concerned with clarifying the asymptotic (long time) value of S_E for both local and nonlocal initial conditions.

C. Asymptotic entanglement from local initial conditions: A simple example

As a simple application, consider the particular localized initial condition

$$|\Psi(0)\rangle = |0\rangle \otimes |L\rangle, \tag{18}$$

which implies $a_k(0)=0$ and $b_k(0)=1$. For this simple case, the spinor components at time t from Eq. (12), have been explicitly calculated in Ref. [10] as

$$\tilde{a}_k(t) = \frac{ie^{ik}}{2\sqrt{1+\cos^2 k}}[e^{-i\omega_k t} - (-1)^t e^{i\omega_k t}],$$

$$\tilde{b}_k(t) = \frac{1}{2}\left(1 + \frac{\cos k}{\sqrt{1+\cos^2 k}}\right)e^{-i\omega_k t} + \frac{(-1)^t}{2}\left(1 - \frac{\cos k}{\sqrt{1+\cos^2 k}}\right)e^{i\omega_k t}. \tag{19}$$

The relevant quantities for the entropy entanglement are A and B, defined in Eqs. (15). After some manipulation, from Eq. (19) we obtain

$$A(t) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{1-(-1)^t \cos(2\omega_k t)}{2(1+\cos^2 k)},$$

$$B(t) = \int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{ie^{ik}}{2\sqrt{1+\cos^2 k}}\left[1 - (-1)^t\left(\frac{\cos(2\omega_k t)\cos k}{\sqrt{1+\cos^2 k}} + i\sin(2\omega_k t)\right)\right]. \tag{20}$$

The time dependence of these expressions vanishes in the long time limit and we obtain the exact asymptotic values

$$\bar{A} = \lim_{t\to\infty} A(t) = \frac{1}{2}\int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{1}{1+\cos^2 k} = \frac{\sqrt{2}}{4},$$

$$\bar{B} = \lim_{t\to\infty} B(t) = \frac{i}{2}\int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{\cos^2 k}{1+\cos^2 k} = i\frac{2-\sqrt{2}}{4}. \tag{21}$$

From Eq. (16), the exact eigenvalues of the reduced density operator are

$$r_1 = \frac{1}{\sqrt{2}} \text{ and } r_2 = 1 - \frac{1}{\sqrt{2}}. \tag{22}$$

These eigenvalues yield the asymptotic value for the entropy of entanglement

$$\bar{S}_0 = \frac{1}{2} + \left(\frac{1}{\sqrt{2}} - 1\right)\log_2(\sqrt{2}-1) \approx 0.87243\cdots. \tag{23}$$

This exact value agrees with the numerical observations reported in Ref. [6] for the case of a Hadamard walk with arbitrary initial coin states and a localized initial position. The analytical procedure outlined above may be repeated for arbitrary initial coin states, with the same result. We include the details of such calculation, done for a generic initial coin state, in the Appendix. The common feature of all localized initial conditions is that their Fourier transforms $\tilde{a}_k(0)$ and $\tilde{b}_k(0)$ are uniform (i.e., k independent) and this determines the asymptotic value of the entropy of entanglement $\bar{S}_E \approx 0.872$.

III. NONLOCAL INITIAL CONDITIONS

Most previous work on quantum walks has dealt with initial wavevectors localized in a position eigenstate $|0\rangle$. When nonlocal initial conditions are considered, new features emerge. Let us consider a quantum walk initialized in a simple uniform superposition of two position eigenstates such as

$$|\Psi_\pm\rangle = \frac{|-1\rangle \pm |+1\rangle}{\sqrt{2}} \otimes |\chi\rangle, \tag{24}$$

where $|\chi\rangle = (|R\rangle + i|L\rangle)/\sqrt{2}$. The entanglement induced by the evolution operator when starting from the initial sates defined in Eq. (24) is shown in Fig. 1. The asymptotic values are $\bar{S}_+ \approx 0.979$ and $\bar{S}_- \approx 0.661$, respectively. This rather large difference is exclusively due to the phase shift $|\Psi_+\rangle \to |\Psi_-\rangle$ alone. On the other hand, a localized initial condition such as

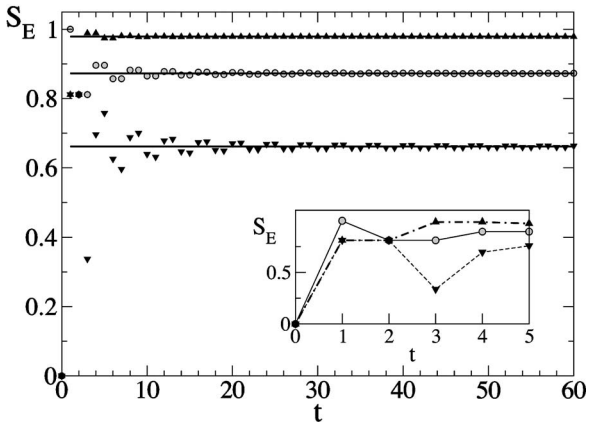

FIG. 1. Evolution of the entropy of entanglement for the initial delocalized sates from Eq. (24) (up and down black triangles, respectively) and for the localized sate from Eq. (25) (gray circles). The time evolution was calculated from Eqs. (30). The horizontal lines represent the asymptotic entanglement levels 0.661, 0.872, and 0.979 obtained from Eqs. (31) as explained in the text. The inset shows the first steps in detail.

$$|\Psi_0\rangle = |0\rangle \otimes |\chi\rangle \tag{25}$$

yields the intermediate value for asymptotic entanglement $S_0 \approx 0.872$ as expected for any localized initial condition (see the previous section, Eq. (23) and Appendix A). Below, we provide an analytical explanation for the observed values in the nonlocal case.

As can be seen in Fig. 1, the rate at which the asymptotic value for entanglement is approached is faster for higher asymptotic entanglement levels. The inset in this figure shows the first five steps in detail. The local initial condition $|\Psi_0\rangle$ is fully entangled ($S_E=1$) after the first time step and reaches its asymptotic level after ~ 10 steps. The nonlocal conditions $|\Psi_\pm\rangle$ have the same evolution for S_E in the first two steps, but the phase difference causes very different entanglement levels after the third time step: $|\Psi_+\rangle$ reaches its asymptotic level after three steps, while $|\Psi_-\rangle$ takes about 30 time steps to stabilize.

A. Asymptotic entanglement

Consider the problem of determining the asymptotic entanglement for nonlocal initial conditions of the form

$$|\Psi(0)\rangle = \sum_x c_x(0)|x\rangle \otimes |\chi\rangle \tag{26}$$

with real $c_x(0)$. The coin state $|\chi\rangle$ in Eq. (26) is such that

$$b_x(0) = ia_x(0) = \frac{c_x(0)}{\sqrt{2}} \text{ or, equivalently, } \tilde{b}_k(0) = i\tilde{a}_k(0). \tag{27}$$

This restriction considerably simplifies the algebra, but it is not essential and the method applies equally well to arbitrary initial coin states.

The eigenvalues of the reduced density operator depend on the real coefficients A, C and on the complex one B, defined in Eqs. (15). Figure 2 shows the entropy of entanglement as a function of these coefficients. Maximum entanglement would be obtained for $A=1/2$ and $B=0$, when the reduced operator corresponds to the minimum information mixture $\rho_c = I/2$.

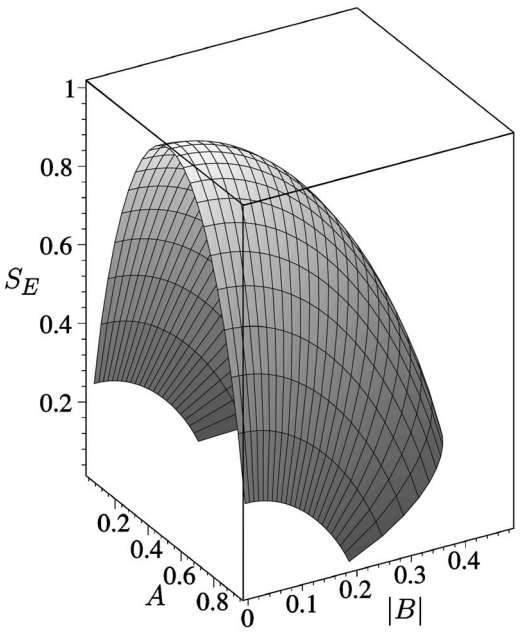

FIG. 2. Entropy of entanglement S_E as a function of A and $|B|$, defined in Eqs. (15).

In order to find expressions for $\bar{A}$ and $\bar{B}$, we start by rewriting Eq. (12) in the more explicit form

$$\tilde{a}_k(t) = \alpha_k^2 F_k v_k e^{-i\omega_k t} + (-1)^t \beta_k^2 G_k w_k e^{i\omega_k t},$$

$$\tilde{b}_k(t) = \alpha_k^2 F_k u_k e^{-i\omega_k t} + (-1)^t \beta_k^2 G_k u_k e^{i\omega_k t}. \tag{28}$$

Here, α_k and β_k are the real, positive functions defined in Eq. (9) and u_k, v_k and w_k, the other part of the eigenvectors of U_k, are defined in Eq. (10). The dependence on the initial conditions is contained in the complex factors

$$F_k \equiv u_k^* \tilde{a}_k(0) + v_k^* \tilde{b}_k(0),$$

$$G_k \equiv u_k^* \tilde{a}_k(0) + w_k^* \tilde{b}_k(0). \tag{29}$$

The required expressions for $|\tilde{a}_k|^2$, $|\tilde{b}_k|^2$, and $\tilde{a}_k \tilde{b}_k^*$ are

$$|\tilde{a}_k(t)|^2 = \alpha_k^4 |F_k|^2 |v_k|^2 + \beta_k^4 |G_k|^2 |w_k|^2 + (-1)^t 2\alpha_k^2 \beta_k^2 \,\mathrm{Re}[F_k G_k^* v_k w_k^* e^{-2i\omega_k t}],$$

$$|\tilde{b}_k(t)|^2 = \alpha_k^4 |F_k|^2 + \beta_k^4 |G_k|^2 + (-1)^t 2\alpha_k^2 \beta_k^2 \,\mathrm{Re}[F_k G_k^* e^{-2i\omega_k t}],$$

$$\tilde{a}_k(t)\tilde{b}_k^*(t) = \alpha_k^4 |F_k|^2 v_k u_k^* + \beta_k^4 |G_k|^2 w_k u_k^* + (-1)^t \alpha_k^2 \beta_k^2 [F_k G_k^* v_k e^{-2i\omega_k t} + F_k^* G_k w_k e^{2i\omega_k t}] u_k^*. \tag{30}$$

In the long-time limit, the contribution of the time-dependent terms in the k integrals of Eqs. (30) vanishes as

$t^{-1/2}$, as shown in detail in Ref. [10]. The asymptotic values $\bar{A}$, $\bar{B}$, and $\bar{C}$ can be obtained from the time-independent expressions

$$\bar{A} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} (\alpha_k^4 |F_k|^2 |v_k|^2 + \beta_k^4 |G_k|^2 |w_k|^2),$$

$$\bar{C} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} (\alpha_k^4 |F_k|^2 + \beta_k^4 |G_k|^2),$$

$$\bar{B} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} (\alpha_k^4 |F_k|^2 v_k u_k^* + \beta_k^4 |G_k|^2 w_k u_k^*), \tag{31}$$

which hold for arbitrary initial conditions.

Now we particularize these expressions for the initial states defined in Eq. (24). Using the symmetry condition, (27), the required squared moduli $|F_k|^2$ and $|G_k|^2$ can be expressed as

$$|F_k|^2 = 4|\tilde{a}_k(0)|^2[1 - \cos(k - \omega_k + \pi/4)],$$

$$|G_k|^2 = 4|\tilde{a}_k(0)|^2[1 + \cos(k + \omega_k + \pi/4)]. \tag{32}$$

Since $\bar{A} + \bar{C} = 1$, we need only perform the integration for $\bar{C}$,

$$\bar{C} = \int_{-\pi}^{\pi} \frac{dk}{2\pi} |\bar{b}_k|^2 \equiv \int_{-\pi}^{\pi} \frac{dk}{2\pi} Q(k) |\tilde{a}_k(0)|^2, \tag{33}$$

where $Q(k)$ is a real function,

$$Q(k) = 4\{\alpha_k^4[1 - \cos(k - \omega_k + \pi/4)] + \beta_k^4[1 + \cos(k + \omega_k + \pi/4)]\} \tag{34}$$

which, after some manipulation, can be simply expressed as

$$Q(k) = 1 + \frac{\sin k \cos k}{1 + \cos^2 k}. \tag{35}$$

Note that this weight function satisfies $Q(k) > 0$ and $\int_{-\pi}^{\pi} (dk/2\pi) Q(k) = 1$.

The asymptotic form for $\bar{B}$ is pure imaginary, so it suffices to calculate the imaginary part of $\bar{B}$,

$$\mathrm{Im}[\bar{B}] = \mathrm{Im}\left[\int_{-\pi}^{\pi} \frac{dk}{2\pi} \overline{a_k b_k^*} \right] \equiv \int_{-\pi}^{\pi} \frac{dk}{2\pi} R(k) |\tilde{a}_k(0)|^2, \tag{36}$$

where $R(k)$,

$$R(k) \equiv 4\sqrt{2}\{\alpha_k^4[1 - \cos(k - \omega_k + \pi/4)]\sin(k - \omega_k) - \beta_k^4[1 + \cos(k + \omega_k + \pi/4)]\sin(k + \omega_k)\} \tag{37}$$

simplifies to

$$R(k) = \frac{\sin^2 k}{1 + \cos^2 k}. \tag{38}$$

This even function satisfies $R(k) \geqslant 0$ and $\int_{-\pi}^{\pi} (dk/2\pi) R(k) = \sqrt{2} - 1$. The required quantity $\bar{S}_E$ can now be evaluated from Eqs. (33) and (36) for different initial conditions satisfying Eq. (27).

For the local initial condition from Eq. (25), we have $|\tilde{a}_k(0)|^2 = 1/2$ and, from Eq. (33), $\bar{A} = \bar{C} = 1/2$ results immediately. In this case, Eq. (16) reduces to $\bar{r}_{1,2} = \frac{1}{2} \pm |\bar{B}|$ and the asymptotic eigenvalues are determined by $|\bar{B}|$ alone. This quantity can be trivially obtained from Eq. (36) as

$$B_0 = |\bar{B}(\Psi_0)| = \frac{\sqrt{2} - 1}{2}. \tag{39}$$

Thus, the asymptotic eigenvalues, $r_1 = 1/\sqrt{2}$ and $r_2 = 1 - 1/\sqrt{2}$, characteristic of localized initial conditions are obtained and the asymptotic entanglement, from Eq. (23), is $\bar{S}_0 \approx 0.872$.

We now return to the case of nonlocal initial conditions $|\Psi_\pm\rangle$ defined in Eq. (24), for which

$$|\tilde{a}_k(0)|^2 = \begin{cases} \cos^2 k & \text{for } |\Psi_+\rangle, \\ \sin^2 k & \text{for } |\Psi_-\rangle. \end{cases} \tag{40}$$

Since $\int_{-\pi}^{\pi} (dk/2\pi) Q(k) \cos^2 k = \int_{-\pi}^{\pi} (dk/2\pi) Q(k) \sin^2 k = \frac{1}{2}$, we obtain from Eq. (33), $A = C = 1/2$ and the eigenvalues are determined by $|B|$ alone. When inserted in Eq. (36), these initial conditions result in

$$B_+ \equiv |\bar{B}(\Psi_+)| = \int_{-\pi}^{\pi} \frac{dk}{2\pi} R(k) \cos^2 k = \frac{(\sqrt{2} - 1)^2}{2},$$

$$B_- \equiv |\bar{B}(\Psi_-)| = \int_{-\pi}^{\pi} \frac{dk}{2\pi} R(k) \sin^2 k = \frac{1}{2} - (\sqrt{2} - 1)^2. \tag{41}$$

Note that these values are related by $B_0 = \frac{1}{2}(B_- + B_+)$. The exact eigenvalues are

$$r_1 = 2 - \sqrt{2}, \quad r_2 = \sqrt{2} - 1 \quad \text{for } |\Psi_+\rangle \tag{42}$$

and

$$r_1 = 2(\sqrt{2} - 1), \quad r_2 = (\sqrt{2} - 1)^2 - 1 \quad \text{for } |\Psi_-\rangle, \tag{43}$$

and the corresponding asymptotic entanglements are,

$$\bar{S}_+ \equiv \frac{1}{\sqrt{2}} - 1 - \log_2(\sqrt{2} - 1) = 0.97866\cdots$$

$$\bar{S}_- \equiv -2(\sqrt{2} - 1)(1 + \sqrt{2}\log_2(\sqrt{2} - 1)) = 0.66129\cdots, \tag{44}$$

respectively. These exact values are coincident with those obtained numerically, see Fig. 1. These are the maximum and minimum possible entanglement levels which can be obtained when starting in the position subspace $\mathcal{H}_1$ spanned by the kets $|-1\rangle$ and $|1\rangle$ with fixed coin. We show below that starting from a generic state in this subspace, all intermediate values of asymptotic entanglement are possible.

B. Generic nonlocal initial state in $\mathcal{H}_1$

Consider a generic ket in $\mathcal{H}_1$ as the initial condition for position. We keep the same initial coin $|\chi\rangle$ which leads to a symmetric evolution in the local case. Thus, we consider initial states of the form

$$|\Psi(\theta,\varphi)\rangle = (\cos\theta|-1\rangle + e^{-i\varphi}\sin\theta|1\rangle)\otimes|\chi\rangle. \quad (45)$$

The parameters $\theta\in[-\pi/2,\pi/2]$ and $\varphi\in[-\pi,\pi]$ are real angles. The initial amplitudes are $\tilde{a}_k(0)=(e^{ik}\cos\theta + e^{-i(k+\varphi)}\sin\theta)/\sqrt{2}$, $\tilde{b}_k(0)=i\tilde{a}_k(0)$ so,

$$|\tilde{a}_k(0)|^2 = |\tilde{b}_k(0)|^2 = \frac{1}{2}[1+\sin(2\theta)\cos(2k+\varphi)]. \quad (46)$$

We use Eq. (33) to obtain,

$$\bar{C} = \frac{1}{2} + \sin(2\theta)\sin(\varphi)\int_{-\pi}^{\pi}\frac{dk}{2\pi}Q(k)\sin(2k)$$

$$= \frac{1}{2} - B_+\sin(2\theta)\sin(\varphi). \quad (47)$$

For arbitrary φ and $\theta=0,\pm\pi/2$ (indicating localized initial positions) or for arbitrary θ and $\varphi=0,\pm\pi$ (indicating relative phases zero or π between initial position eigenstates) we have $\bar{A}=\bar{C}=1/2$ and the asymptotic entropy is determined by the value of $|\bar{B}|$ alone.

$|\bar{B}|$ is obtained from Eq. (36), which can be decomposed as

$$\mathrm{Im}[\bar{B}] = B_0 - B'\sin(2\theta)\cos(\varphi), \quad (48)$$

with B_0 defined in Eq. (39) and

$$B' \equiv \frac{B_- - B_+}{2} = \frac{3\sqrt{2}-4}{2}. \quad (49)$$

The range of variation of $|\bar{B}|$ is determined by B'. The maximum $|\bar{B}|_{\max}=B_0+B'=B_-$ results in minimum entanglement. It is obtained either for $(\theta,\varphi)=(-\pi/4,0)$ or $(\theta,\varphi)=(\pi/4,\pm\pi)$, both cases correspond to a uniform superposition of position eigenstates with a π phase difference, i.e., the case $|\Psi_-\rangle$, discussed previously. The minimum value, $|\bar{B}|_{\min}=B_0-B'=B_+$, is obtained either for $(\theta,\varphi)=(\pi/4,0)$ or $(\theta,\varphi)=(-\pi/4,\pm\pi)$, leads to the maximum entanglement and corresponds to a uniform superposition with equal phases, as in $|\Psi_+\rangle$. For $\theta=0,\pm\pi/2$, corresponding to localized initial conditions, the intermediate value $|\bar{B}|=B_0$, leading to $\bar{S}_0\approx 0.872$, is obtained. The asymptotic eigenvalues $\bar{r}_{1,2}$ can be obtained from Eq. (16), as

$$\bar{r}_{1,2}(\theta,\varphi) = \frac{1}{2} \pm \{[B_0 - B'\sin(2\theta)\cos(\varphi)]^2 + B_+^2\sin^2(2\theta)\sin^2(\varphi)\}^{1/2} \quad (50)$$

and the asymptotic entanglement $\bar{S}_E(\theta,\varphi)$ can be evaluated exactly from Eq. (17), as shown in Fig. 3.

A contour plot of this surface, Fig. 4, shows that there are only two maximum and two minimum points (for initial conditions $|\Psi_+\rangle$ and $|\Psi_-\rangle$) for which the asymptotic entanglements are $\bar{S}_+\approx 0.979$ and $\bar{S}_-\approx 0.661$, respectively. The vertical dashed lines indicate initially localized positions, where the entanglement is $\bar{S}_0\approx 0.872$. The asymptotic entanglement corresponding to initial conditions given by Eq. (50) with $\varphi=0$, is shown in Fig. 5. The relative phase between initial position eigenstates can be chosen so that the asymptotic entanglement is the same as in the localized case. This is the case for relative phases $\varphi=\pm\pi/2$ corresponding to initial positions of the form $|\Psi_1\rangle=(\cos\theta|-1\rangle\pm i\sin\theta|1\rangle)\otimes|\chi\rangle$ (indicated by the horizontal dashed lines in Fig. 4), as can be seen by inspection of Eq. (50).

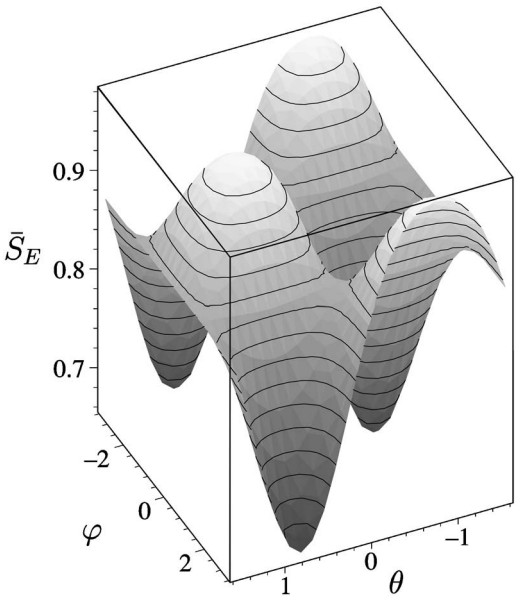

FIG. 3. Asymptotic entropy of entanglement $\bar{S}_E(\theta,\varphi)$ as a function of the initial state from Eq. (45). The entropy is calculated from the expressions for $\bar{C}$ and $|B|$ given in Eqs. (47) and (48).

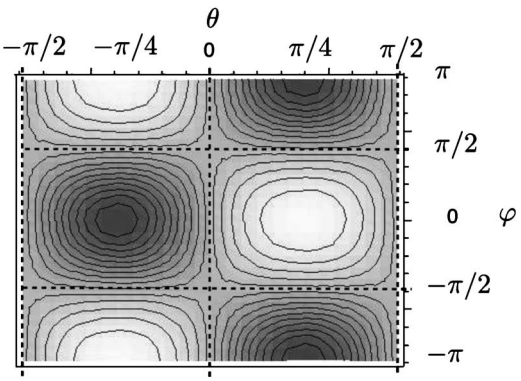

FIG. 4. Contour plot the surface shown in Fig. 3. Clear areas indicate maxima and dark areas, the minimum values. The vertical dashed lines correspond to localized initial conditions and the horizontal dashed lines to states proportional to $\cos\theta|-1\rangle\pm i\sin\theta|1\rangle$. In both cases, they result in an asymptotic entanglement $\bar{S}_0\approx 0.872$.

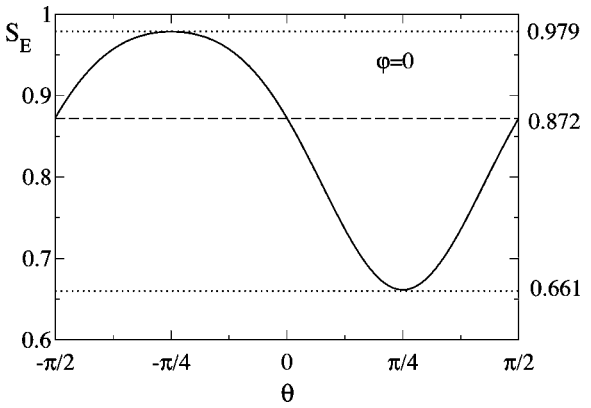

FIG. 5. Asymptotic entropy of entanglement $\bar{S}_E(\theta,\varphi=0)$ for initial states in $\mathcal{H}_1$ (see Eq. (45)). This curve has been generated substituting the eigenvalues given by Eq. (50), with $\varphi=0$, into Eq. (17). The maximum and minimum values (dotted lines) can be calculated with arbitrary precision from the exact eigenvalues given in Eqs. (42) and Eqs. (43). The dashed line indicates the level of asymptotic entanglement associated to local initial conditions.

C. More general nonlocal initial states

In order to further illustrate the effects that the nonlocality in the initial condition can have on the asymptotic entanglement level, we consider an initial Gaussian wave packet with a characteristic spread $\sigma \gg 1$ in position space with the same coin state $|\chi\rangle$ as before. In this case, the Fourier transformed coefficients $\tilde{a}_k(0) \propto \sqrt{\sigma} e^{-k^2\sigma^2/2}$ correspond to a well-localized state in k space with $\lim_{\sigma\to\infty}|\tilde{a}_k(0)|^2 = 2\pi\delta(k)$, where $\delta(k)$ is Dirac's delta function. In this limit, the elements of the asymptotic reduced density matrix can be trivially evaluated from Eqs. (33) and (36)

$$\bar{C} = \lim_{\sigma\to\infty} \int_{-\pi}^{\pi} \frac{dk}{2\pi} Q(k)|\tilde{a}_k(0)|^2 = Q(0) = 1,$$

$$\mathrm{Im}[\bar{B}] = \lim_{\sigma\to\infty} \int_{-\pi}^{\pi} \frac{dk}{2\pi} R(k)|\tilde{a}_k(0)|^2 = R(0) = 0,$$

the eigenvalues are $r_1=1$ and $r_2=0$ and the corresponding asymptotic entropy of entanglement vanishes.

This simple example shows that for a particular uniform distribution in position space, a product state results in the long time limit. Of course, this is not true for arbitrary relative phases between the initial position eigenstates. However, it is clear that if more nonlocality is introduced in the initial condition and the appropriate relative phases are chosen, lower asymptotic entanglement levels may be obtained, until eventually a product state is reached. A more detailed analysis of this example shows that for $\sigma \gg 1$, the smaller eigenvalue approaches zero as $(2\sigma)^{-4}$ and the asymptotic entropy of entanglement decays as $\bar{S}_E \sim \log_2 \sigma/4\sigma^4 + O(\sigma^{-8})$. Thus, for $\sigma \gtrsim 10$ the asymptotic entanglement is already quite small, $S_E \approx 10^{-4}$. If many sites are initially occupied, the entanglement level at long times becomes negligible.

IV. CONCLUSIONS

The long-time (asymptotic) entanglement properties of the Hadamard walk on the line are analytically investigated using the Fourier representation. The von Neumann entropy of the reduced density operator is used to quantify entanglement between the coin and position degrees of freedom. The fact that the evolution operator of a quantum walk is diagonal in k space allows us to obtain clean, exact expressions for the asymptotic entropy of entanglement, $\bar{S}_E$ for different classes of initial conditions.

The exact value of asymptotic entanglement for local initial conditions $\bar{S}_0=0.87243\ldots$, is analytically obtained for two different initial coins $|L\rangle$ and $|R\rangle+i|L\rangle$. In Appendix A, we apply the same method to generic initial coin states and show that for local initial states they do not affect the asymptotic entanglement level. This is consistent with the results of the numerical exploration reported in Ref. [6].

Asymptotic entanglement levels for nonlocal initial conditions are reported for the first time in the context of the Hadamard walk on the line. In order to show that the asymptotic entanglement level is strongly dependent on whether the initial condition is localized or delocalized in position space, we apply our analytical method to consider in detail the case of initial conditions in the position subspace $\mathcal{H}_1$ spanned by $|\pm 1\rangle$, with a fixed coin $|\chi\rangle=|R\rangle+i|L\rangle$. An exact expression for the asymptotic entanglement entropy has been obtained and it shows that the asymptotic entanglement level varies smoothly between the extreme values $\bar{S}_- \approx 0.661$ and $\bar{S}_+ \approx 0.979$. As expected, for the localized initial positions $|\pm 1\rangle$ it reduces to $\bar{S}_0=0.872\ldots$, but some superpositions with the particular relative phases $\pm\pi/2$ also result in this intermediate entanglement level. In order to explore the effect of further nonlocality on the asymptotic entanglement the case of an initial Gaussian profile in position space, with characteristic spread $\sigma \gg 1$, is considered. For the particular phase relation considered, the resulting asymptotic entanglement decays fast with increasing initial nonlocality. Thus, if many sites are initially occupied, negligible entanglement may be obtained at long times.

The results presented in this work certainly need to be extended to less simple systems. Most likely, quantum walks with either more particles, more dimensions or both will be needed to be useful for algorithmic applications. The problem of entanglement in such systems is more involved. For example, in a quantum walk with two noninteracting particles there are four kinds of degrees of freedom and several kinds of entanglement may coexist. At some point in the evolution, a measurement of the position of one particle will affect the probability distribution of the other in a way which depends on the kinds and levels of entanglement present at that time. Some initial work in this direction is presently under way.

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APPENDIX: INDEPENDENCE OF THE ASYMPTOTIC ENTANGLEMENT LEVEL OF INITIALLY LOCALIZED POSITION EIGENSTATES ON THE INITIAL COIN

In this Appendix we provide an analytical proof of the fact that the asymptotic entanglement level does not depend on the initial coin state for initially localized position eigenstates. As mentioned in the main text, a numerical study reported in Ref. [6] has already reached this result.

Consider as an initial condition a position eigenstate, which we take, without loss of generality, as $x=0$. Let us also consider a generic coin

$$|\Psi(0)\rangle = |0\rangle \otimes \frac{1}{\sqrt{2}}(\cos\alpha|R\rangle + e^{i\beta}\sin\alpha|L\rangle), \tag{A1}$$

where α,β are two real angles. The Fourier-transformed initial coefficients, Eq. (6), are

$$\tilde{a}_0(0) = a_0(0) = \cos\alpha,$$

$$\tilde{b}_0(0) = b_0(0) = e^{i\beta}\sin\alpha. \tag{A2}$$

From expressions (29), for this class of initial conditions we obtain

$$\begin{aligned}|F_k|^2 &= \cos^2\alpha + |v_k|^2\sin^2\alpha + \sin(2\alpha)\mathrm{Re}[u_k^* v_k e^{-i\beta}]\\ &= F_e(k) + F_o(k),\end{aligned}$$

$$\begin{aligned}|G_k|^2 &= \cos^2\alpha + |w_k|^2\sin^2\alpha + \sin(2\alpha)\mathrm{Re}[u_k^* w_k e^{-i\beta}].\\ &= G_e(k) + G_o(k),\end{aligned} \tag{A3}$$

where the even and odd parts are the real functions

$$\begin{aligned}F_e(k) &\equiv \cos^2\alpha + |v_k|^2\sin^2\alpha\\ &\quad - [1-\sqrt{2}\cos(\omega_k - k)]\sin(2\alpha)\cos\beta,\end{aligned}$$

$$F_o(k) \equiv -\sqrt{2}\sin(\omega_k - k)\sin(2\alpha)\sin\beta,$$

$$\begin{aligned}G_e(k) &\equiv \cos^2\alpha + |w_k|^2\sin^2\alpha\\ &\quad - [1+\sqrt{2}\cos(\omega_k + k)]\sin(2\alpha)\cos\beta,\end{aligned}$$

$$G_o(k) \equiv -\sqrt{2}\sin(\omega_k + k)\sin(2\alpha)\sin\beta. \tag{A4}$$

The eigenvalues (16) of the reduced density operator, which determine the entanglement level, depend only on its determinant

$$\Delta = AC - |B|^2 = C - (C^2 + |B|^2). \tag{A5}$$

The asymptotic entanglement will be independent of the initial coin state if $\bar{\Delta}$ does not depend on α or β. From the general asymptotic expressions (31) which are valid in the long-time limit for arbitrary initial conditions, we obtain

$$\bar{C} = c_1 + (c_2 - c_1)\sin^2\alpha + c_3\sin(2\alpha)\cos\beta,$$

$$\bar{B} = b_1 + (b_2 - b_1)\sin^2\alpha + \sin(2\alpha)(b_3\cos\beta + ib_4\sin\beta), \tag{A6}$$

where the real coefficients c_j, b_j are explicitly

$$c_1 = \int_{-\pi}^{\pi}\frac{dk}{2\pi}(\alpha_k^4 + \beta_k^4) = 1 - \frac{\sqrt{2}}{4},$$

$$c_2 = \int_{-\pi}^{\pi}\frac{dk}{2\pi}(\alpha_k^4|v_k|^2 + \beta_k^4|w_k|^2) = \frac{\sqrt{2}}{4},$$

$$\begin{aligned}b_1 = c_3 &= -\int_{-\pi}^{\pi}\frac{dk}{2\pi}\{\alpha_k^4[1-\sqrt{2}\cos(\omega_k - k)]\\ &\quad + \beta_k^4[1+\sqrt{2}\cos(\omega_k + k)]\}\\ &= \frac{1}{2} - \frac{\sqrt{2}}{4},\end{aligned}$$

$$\begin{aligned}b_2 &= -\int_{-\pi}^{\pi}\frac{dk}{2\pi}\{\alpha_k^4|v_k|^2[1-\sqrt{2}\cos(\omega_k - k)]\\ &\quad + \beta_k^4|w_k|^2[1+\sqrt{2}\cos(\omega_k + k)]\}\\ &= \frac{\sqrt{2}}{4} - \frac{1}{2},\end{aligned}$$

$$\begin{aligned}b_3 &= -\int_{-\pi}^{\pi}\frac{dk}{2\pi}\{\alpha_k^4[1-\sqrt{2}\cos(\omega_k - k)^2]^2\\ &\quad + \beta_k^4[1+\sqrt{2}\cos(\omega_k + k)]^2\}\\ &= \frac{\sqrt{2}}{4} - \frac{1}{2},\end{aligned}$$

$$\begin{aligned}b_4 &= 2\int_{-\pi}^{\pi}\frac{dk}{2\pi}[\alpha_k^4\sin^2(\omega_k - k) + \beta_k^4\sin^2(\omega_k + k)]\\ &= \frac{\sqrt{2}-1}{2}.\end{aligned} \tag{A7}$$

These coefficients can be conveniently expressed in terms of one of them, i.e., b_1, since they satisfy the relations

$$c_1 = 1 - c_2 = \frac{1}{2} - b1,$$

$$b_2 = b_3 = -b_1,$$

$$b_4 = \sqrt{2}b_1.$$

Thus, Eqs. (A6) can be written as

$$\bar{C} = b_1[3 + \sqrt{2} - 2\sin^2\alpha + \sin(2\alpha)\cos\beta],$$

$$\bar{B} = b_1[1 - 2\sin^2\alpha + \sin(2\alpha)(-\cos\beta + i\sqrt{2}\sin\beta)]. \tag{A8}$$

Using these expressions in Eq. (A5), it is simple to check that the α and β dependence cancels out and only the independent terms in $\bar{C}$ and $\bar{B}$ contribute to the eigenvalues. The resulting exact determinant is, from Eq. (A5),

$$\bar{\Delta} = c_1(1 - c_1) - b_1^2 = c_2(1 - c_2) - b_2^2 = \frac{\sqrt{2} - 1}{2}. \tag{A9}$$

From this simple expression we obtain the eigenvalues

$$r_{1,2} = \frac{1}{2}(1 \pm \sqrt{1 - 4\bar{\Delta}}) = \begin{cases} 1/\sqrt{2}, \\ 1 - 1/\sqrt{2} \end{cases}$$

which, as mentioned in the main text, produce the asymptotic entanglement entropy $\bar{S}_0 = -r_1 \log_2 r_1 - r_2 \log_2 r_2 = 0.872\ldots$.

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