Superdiffusivity of quantum walks: A Feynman sum-over-paths description

F. M. Andrade\textsuperscript{1} and M. G. E. da Luz\textsuperscript{2}

\textsuperscript{1}Departamento de Matemática e Estatística, Universidade Estadual de Ponta Grossa, 84030-900 Ponta Grossa-PR, Brazil
\textsuperscript{2}Departamento de Física, Universidade Federal do Paraná, C.P. 19044, 81531-980 Curitiba-PR, Brazil

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Quantum walks constitute important tools in different applications, especially in quantum algorithms. To a great extent their usefulness is due to unusual diffusive features, allowing much faster spreading than their classical counterparts. Such behavior, although frequently credited to intrinsic quantum interference, usually is not completely characterized. Using a recently developed Green’s function approach [Phys. Rev. A \textbf{84}, 042343 (2011)], here it is described – in a rather general way – the problem dynamics in terms of a true sum over paths history a la Feynman. It allows one to explicitly identify interference effects and also to explain the emergence of superdiffusivity. The present analysis has the potential to help in designing quantum walks with distinct transport properties.

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I. INTRODUCTION

Quantum walks (QWs), a quantum version of classical random walks (CRWs) \textsuperscript{1}, is a relatively simple class of systems, yet containing almost all the essential aspects of quantum mechanics \textsuperscript{2, 3}. They can be used to model a large number of phenomena \textsuperscript{4, 5}, such as: energy transport in biological systems \textsuperscript{6}; Bose-Einstein condensates redistribution \textsuperscript{7}; quantum phase transition in optical lattices \textsuperscript{8}; and decoherence processes \textsuperscript{9}. But, certainly where QWs have attracted more interest is in quantum computing \textsuperscript{10, 11}. In fact, QWs allow the development of new quantum algorithms \textsuperscript{12}, which often display much better performance than their classical siblings \textsuperscript{12, 13}.

QWs usefulness in applications is in great part due to their unusual transport properties. For instance, they present exponentially faster hitting times \textsuperscript{14, 16} (the time necessary to visit any vertex in the system graph space), an important feature for searching in discrete databases \textsuperscript{17, 18}. Such faster spreading compared to CRWs \textsuperscript{2} is usually attributed to interference \textsuperscript{2, 19}, a key ingredient in implementations \textsuperscript{20, 21} and believed central to explain distinct behaviors \textsuperscript{22}. However, exactly how these effects emerge in QWs usually is not totally characterized \textsuperscript{24}, posing challenges as to how one could properly link the high degree of entanglement in QWs \textsuperscript{24} with interference. Furthermore, since interference actually comes from a high proliferation of paths (after all, QWs are associated to the idea of CRWs \textsuperscript{25}), it also bears on the problem of how decoherence \textsuperscript{26} can make the “quantum trajectories” to become classical \textsuperscript{27}.

In trying to understand interference in QWs, a path integral-like treatment would be appropriate. Actually, a few interesting works along this line have been proposed \textsuperscript{28}. However, they address the problem from a different perspective, using combinatorial analysis to compute final states \textsuperscript{24}, but not considering intermediary steps in terms of Feynman’s history of trajectories \textsuperscript{30}. Hence, interference is not made truly explicit.

In the present work we show how quantum interference determines QWs uncommon diffusive properties. To this end, the exact Green’s function \textsuperscript{31} – given as a general sum of paths – is written in a closed analytical form. Then, we describe how to calculate relevant quantities in a way identifying the trajectories superposition contributions. To concretely illustrate the approach, we show that the usually observed: (a) complicated oscillatory behavior of the probability distribution for visits at different sites; and (b) the process dispersion dependence on time; are associated to the complex multiple reflections and transmission patterns of the system evolved paths.

Finally, we mention some important technical aspects. There are several ways to formulate QWs, all defined in discrete spaces (graphs) \textsuperscript{2}. Also, time may be either a continuous \textsuperscript{14} or a discrete variable. In the latter, the major formulations are coined \textsuperscript{32} and scattering \textsuperscript{33} QWs. Continuous time and coined are related through appropriate limits \textsuperscript{34}, whereas coined and scattering are unitarily equivalent in any topology and for arbitrary transition amplitudes \textsuperscript{35}. Hence, we consider only scattering quantum walks (SQWs), keeping in mind that our finds can be extended to such other constructions as well. Moreover, the Green’s function method considered here \textsuperscript{31} is valid for any graph topology. Although for our purposes we address QWs on the line, avoiding extra and unnecessary mathematical complications, we mention that the same type of analysis would likewise work in more complex networks.

II. THE SUM OVER PATHS DESCRIPTION

We assume an undirected 1D lattice of equally spaced vertices labeled in Z, Fig. 1. Pairs of neighbor vertices...
includes both cases once the vertex dependent scattering quantum amplitudes.

are joined by a single edge. To each edge we ascribe two positions of the initial and final, \( i \) and \( f \), edges. FIG. 2. For \( G \), the three possible situations for the relative positions of the initial and final, \( i \) and \( f \), edges.

are joined by a single edge. To each edge we ascribe two basis states. For instance, in Fig. 1 for the edge between \( j-1 \) and \( j \) (and \( j+1 \)) we have \(|j, j+1\rangle\) and \(|j+1, j\rangle\) \((= \langle j+1, j |)\). Therefore, the full set \(|\{j, j\}\rangle\) spans all the possible system states \(|\psi\rangle\). The quantum numbers \( \sigma = \pm 1 \) (hereafter for short \( \pm \)) represent the propagation direction along the lattice (or graph). The discrete dynamics is given by the one step time evolution operator \( U \), such that the state at times \( m+1 \) and \( m \) are related by \(|\psi(m+1)\rangle = U|\psi(m)\rangle\). For an arbitrary phase \( z = \exp(\gamma r) \), we have \( U|\sigma, j\rangle = z^* \left( t^{(\sigma)}_{j} |\sigma, j - \sigma\rangle + t^{(-\sigma)}_{j} |j, j - \sigma\rangle \right) \),

\[
U|\sigma, j\rangle = z \left( t^{(\sigma)}_{j} |\sigma, j + \sigma\rangle + t^{(-\sigma)}_{j} |j, j + \sigma\rangle \right). \quad (1)
\]

Here \( r_j \) \((0 \leq r_j, t_j \leq 1 \) and \( 0 \leq \phi^{(\pm)}_{r}, \phi^{(\pm)}_{t} \leq 2\pi) \)

\[
r_j^2 + t_j^2 = 1, \quad \phi^{(+)}_{r} + \phi^{(-)}_{r} = \phi^{(+)}_{t} + \phi^{(-)}_{t} = \pi, \quad t_j^2 = t_j \exp[2\phi^{(\pm)}_{r},] \quad r_j^2 = r_j \exp[2\phi^{(\pm)}_{t}],
\]

guarantee the evolution unitarity. The \( r \)'s and \( t \)'s can be understood as the vertices reflection and transmission quantum amplitudes (see Fig. 1).

The problem is fully described by the Green's function approach in \( \Phi \). Consider the walk starting at the edge \( i \) (between the vertices \( j-1 \) and \( j \)) with the state \( \sigma \) and finally getting to the edge \( f \) (between the vertices \( j+1 \) and \( j+2 \)), for any \( n = 0, 1, 2, \ldots \). The three possible situations are illustrated in Fig. 2. Then, the most general exact expression for the Green's function, representing the transmission probability amplitude \( |\sigma, i \rangle \rightarrow |f \rangle \) reads \(|s = -1 \langle +1| \) in short \( \mp \) for \( f \) to the right (left) of \( i \) and \( s = 0 \) for \( f \) equal to \( i \)

\[
G_{f, \{\sigma, i\}} = \frac{\left( z^{(3+s+\sigma)/2} R^{(s)}_{j-1} + (s+\sigma)/2 \right) T^{(-s)}_{j-(s+1)/2} |\sigma\rangle^{\mp} + z R^{(-s)}_{j-s(n-1)} T^{(s)}_{j-(s-n)} |\sigma\rangle^{\pm} - |s\rangle \left( z^{2} R^{(s)}_{j-s(n-1)/2} T^{(-s)}_{j-s(n-1)/2} + T^{(s)}_{j-s(n-1)/2} \right)}{1 - z^{2} R^{(s)}_{j-s(n-1)} T^{(s)}_{j-s(n-1)}}. \quad (3)
\]

The composed coefficients \( R^{(\pm)}_{j} \) and \( T^{(\pm)}_{j} \), functions of the individual amplitudes \( r^{(\pm)}_{j} \)'s and \( t^{(\pm)}_{j} \)'s, are obtained from the following recurrence relations \( \Phi \) \((\mu_{-} = j - (s+1)(n-1)/2 \) and \( \mu_{+} = j - 1 - (s+1)n/2 \) for \( s \neq 0) \)

\[
R^{(\pm)}_{j} = r^{(\pm)}_{j} + \frac{z^{2} r^{(\pm)}_{k} T^{(\pm)}_{k+1}}{1 - z^{2} r^{(\pm)}_{k} T^{(\pm)}_{k+1}}, \quad R^{(+)}_{j} = T^{(-)}_{j} + \frac{z^{2} t^{(+)}_{k} T^{(-)}_{k+1}}{1 - z^{2} t^{(+)}_{k} T^{(-)}_{k+1}}. \quad (4)
\]

In Eq. 4 it is not specified what is the final direction quantum number, \( \nu \), when arriving at \( f \). In fact, it includes both cases once \( \nu = \sigma (-\sigma) \) corresponds to the term \( 1 (zR) \) in the second \((\ldots)\) in the numerator of Eq. 3. There are different contexts for which we may seek the amplitude transition \( |\sigma, i \rangle \rightarrow |f \rangle \). Common ones are: (i) exactly after \( m = M \) time steps; and (ii) when the system never visits vertices further to the left and to the right than, respectively, \( j = j_{l} \) and \( j = j_{r} \) \((\varepsilon, \text{e.g., for first passage time calculations})\). In both we just need two extra relations for Eq. 3: \( R^{(+)}_{j} = r^{(+)}_{j} \) and \( R^{(-)}_{j} = r^{(-)}_{j} \). Moreover, for (i) we have \( j_{l} = (j-1) - [(M + \delta_{1} - \delta_{1} s)/2 \) and \( j_{r} = j + [(M - \delta_{1} s - 1)/2 \), with \( [x] \) the integer part of \( x \) and \( n \) taken consistently. Finally, for Eq. 3 obviously \( |\psi(0)\rangle = |\sigma, j + (s-1)/2 \rangle \). For \( |\psi(0)\rangle = \sum c_{\sigma, j} |\sigma, j\rangle \), the correct Green's function would be \( G = \sum c_{\sigma, j} G_{f, \{\sigma, i\}} \).

The above exact expression is derived from a sum over infinite many “scattering paths” \( \Phi, \Phi \), starting and ending at the edges \( i \) and \( f \). Its advantage is that
all the possible quantum walk trajectories are "compacted" into a closed formula. So, distinct interference phenomena can be extract from \(G\). Indeed, as demonstrated in \([31]\), this is achieved in a rather systematic way by means of two differential operators. The probability for \(\{\sigma,i\} \rightarrow f\) in exactly \(m\) time steps is given by \(P_{\{\sigma,i\} \rightarrow f}(m) = |\hat{S}_m G_{f,\{\sigma,i\}}|^2\), with \(\hat{S}_m = \frac{1}{2m} \frac{\partial^m}{\partial r_j^m}\) the Step Operator. To see this, we note that \([31]\) \(\hat{S}_m G_{f,\{\sigma,i\}} = \sum_{\nu,p} P_{\nu,p}\), for each \(P_{\nu,p}\) being the contribution of a trajectory from \(i\) to \(f\) in \(m\) steps \([38]\). Interference comes into play when we take the modulus square of such expansion. Also, any specific \(P\) follows from \(P_{\nu}G\), for the Path Operator (superscripts \(\pm\) omitted for clarity)

\[
P_{P} = \prod_{k,l \in P} \frac{t_k^{m_k} r_l^{m_l}}{m_k! m_l!} \left| \left( \frac{\partial^{m_k}}{\partial t_k^{m_k}} \frac{\partial^{m_l}}{\partial r_l^{m_l}} \right) \right|_{r_j,t_j=0,\nu,j}.
\]  

In Eq. \(\text{5}\) the \(t_k\)'s and \(r_l\)'s are the scattering amplitudes (appearing \(m_k\) and \(m_l\) times) characterizing the path associated to \(\nu\) \([31]\).

With this mathematical ‘machinery’, below we can make an analysis of sum over paths for QWs.

\section{III. RESULTS AND DISCUSSION}

Suppose the initial state \(|\psi(0)\rangle = |\sigma,j\rangle\), so we write

\[
U^m |\psi(0)\rangle = |\psi(m)\rangle = z^m \sum_{j'=j-m}^{j+m} \sum_{\nu=\pm} a_{\nu,j'} |\nu,j'\rangle. \tag{6}
\]

Above, some \(a\)'s are zero since certain basis states are absent, e.g., \(|-j,j+m-1\rangle\) cannot be reached in \(m\) steps. In fact, exactly \(2m\) \(a\)'s are not null.

Next, to make contact with CRWs, we observe that by leaving from the edge corresponding to \(\{\sigma,j\}\) there is a determined number of trajectories (eventually none) finally getting to specific edges in exact \(m\) steps. Thus, the total number of paths ending up in any possible \(|\nu,j'\rangle\) is \(2^m\). Since \(p = |a|^2\), the \(a\)'s can be given as the sum of the quantum amplitudes \([38]\) of all paths yielding \(\{\sigma,j\} \rightarrow \{\nu,j'\}\).

As an simple example, for \(|\psi(0)\rangle = |+,j\rangle\) the Fig. \(\text{3}\) schematically illustrates the basis states expansion of \(|\psi(m)\rangle\) (up to \(m = 5\)). Consider \(m = 2\), then

\[
z^{-2} |\psi(2)\rangle = z^{-2} U^2 |+,j\rangle = a_{+,j-2} |-,j-2\rangle + a_{-,j-2} |+,j-2\rangle + a_{-,j-1} |-,j\rangle + a_{+,j+2} |+,j+2\rangle.
\]  

The presence of, say, \(|-,j-2\rangle\) in the expression for \(|\psi(2)\rangle\), Eq. \(\text{7}\), is represented in the \(m = 2\) case of Fig. \(\text{3}\) by an arrow pointing to the vertex \(j - 2\). Moreover, its number, here just a single arrow, means there is only one path getting to \(|-,j-2\rangle\) from \(|+,j\rangle\) if \(m = 2\): a trajectory which initially heading right at \(j\) (since \(|\psi(0)\rangle = |+,j\rangle\), reverses its direction at \(j\), goes to \(j - 1\) (first step), and finally goes to \(j - 2\) (second step), now heading left. Note that in terms of a quantum scattering process, it represents a reflection from the vertex \(j (r_{j+1}^{(+)}\) and then a transmission through the vertex \(j - 1 (t_{j-1}^{(+)})\).

By applying \(\hat{S}_m\) on \(G_{\{\nu,j'\},\{\sigma,j\}}\) and afterwards simply setting \(r_{j+2}^{(\pm)} = t_{j+1}^{(\pm)} = 1 \forall j\), one directly finds that the number of paths leading to \(\{\sigma,j\} \rightarrow \{\nu,j'\}\) after \(m\) steps is given by the binomial coefficient \(39\)

\[
N_{\nu,j'} = \binom{m - 1}{\frac{m + j' - j}{2} - \delta_{\nu j}}. \tag{8}
\]

As a simple check, one can test Eq. \(\text{8}\) with the schematics in Fig \(\text{3}\). Moreover, from the mapping between SQWs and coined QWs in \([33]\), the number of paths to a given \(j'\) state for the latter QW formulation is trivially derived from \(N_{\nu,j'}\) as

\[
N_{j'}^{\text{coined}} = \sum_{\nu} N_{\nu,j'} = \left( \frac{m}{2} \right) \binom{m + j' - j}{m - j' + j} = \left( \frac{m}{2} \right) \binom{m + j' - j}{m - j' + j}, \tag{9}
\]

which agrees with the formula in Ref. \([40]\) (with \(j = 0\)).

Assume any path taking, regardless the order, \(d^{(-)}\) \((d^{(+)}\) steps to the left (right). It would lead the system to \(|\nu,j' = j + d^{(+)} - d^{(-)}\rangle\). Reversing this reasoning, consider a fixed \(m = d^{(+)} + d^{(-)} \geq |\Delta j|\), with \(\Delta j = j' - j\). Paths for which \(d^{(\pm)} = (m \pm \Delta j)/2\) are both integers will result in \(j \rightarrow j'\). To obtain all such paths, we should consider \(G\) for \(J_l = j - d^{(-)}\) and \(J_r = j + d^{(+)}\). The contribution from each path to a given coefficient in Eq. \(\text{9}\) will involve exactly \(m\) position dependent amplitudes \(r_{j+1}^{(\pm)}\)’s and \(t_{j-1}^{(\pm)}\)’s. In this way, the actual procedure to calculate the \(a\)'s is to compute \(a_{\nu,j'} = \hat{S}_m G_{\{\nu,j'\},\{\sigma,j\}}\), for \(J_l, J_r, d^{(\pm)}\) as above.

For complete arbitrary \(r_{j+1}^{(\pm)}\)’s and \(t_{j-1}^{(\pm)}\)’s and for \(m\) in the hundreds, any available computer algebra system can be used to obtain the \(a\)'s as explained. Actually, vertex-dependent quantum amplitudes can give rise to a great

\begin{figure}[h]
\begin{center}
\includegraphics[width=0.8\textwidth]{fig3}
\end{center}
\caption{For each \(m\), an arrow \(\rightarrow (+)\) pointing to the vertex \(j'\) indicates that the basis state \(|+,j'\rangle\) \((-,-j'\rangle\) is present in the expression for \(|\psi(m)\rangle = U^m |+,j\rangle\). The number of arrows of a given type equals the number of distinct paths leading to the corresponding \(|\nu,j'\rangle\).}
\end{figure}
diversity of diffusive properties. So, the present procedure may be useful to test distinct QWs models transport features, helping to choose sets of $i_j^{(+)}$s and $j_j^{(+)}$s more appropriate in different applications (examples to appear elsewhere).

However, a real surprise is for the situation when superdiffusion takes place even for $j$ independent quantum amplitudes and when at each single step the QW resembles an unbiased classical walk (i.e., 50–50% probability to go right-left). In the following, we show how interference can fully explain this apparently non-intuitive behavior.

For $r_j^{(±)} = r_j^{(±)}$, $t_j^{(±)} = t_j^{(±)}$ and from the above prescription, we get ($n_{sup} = \min\{d(\sigma) - \delta_{\sigma}, d(-\sigma) - 1\}$)

$$a_{\nu,j'} = \sum_{n=n_{sup}} \sum_{n=\delta_{\sigma}} f_n C_n,$$

$$C_n = \left[d(\sigma)\right]_{n+1} - \left[d(-\sigma)\right]_{n+1},$$

where $f_n$ gives the number of distinct paths yielding a same amplitude $C_n$ to the $a$’s. This is possible because different paths correspond to a different order of scattering processes along the lattice. Nevertheless, if the final set of scattering’s coincides, the resulting amplitudes $C_n$ are equal. The total number of paths for $a_{\nu,j'}$ is $N_{\nu,j'} = \sum_n f_n = \left(d(\sigma) - \delta_{\sigma}\right)$, which agrees with Eq. (3).

Particularly important in Eq. (11) is the factor $(-1)^n$, arising from the phases difference, Eq. (2), between reflections and transmissions in a trajectory. In fact, for each path the number of directions change along the way is $2n + 1 + \delta_{\sigma}$, Therefore, distinct paths may contribute with distinct signals (through $(-1)^n$) to the sum in Eq. (10), leading to constructive or destructive interference.

Lastly, in the “unbiased” case of $r = t = 1/\sqrt{2}$, i.e., 50%–50% reflection-transmission probability in each vertex (for a similar coined case see, e.g., [40]), Eq. (10) reduces to

$$a_{\nu,j'} = \exp[i\phi] \sum_{n=0}^{d(\sigma)} \left(\frac{r}{t}\right)^{2n+1} (-1)^n,$$

with $\phi$ a global phase (unimportant here) which depends on $j$, $j'$, $\sigma$, $\nu$, $m$ and $\phi^{(±)}_{\nu,t}$. In Eq. (11), $f_n$ gives the number of distinct paths yielding a same amplitude $C_n$ to the $a$’s. This is possible because different paths correspond to a different order of scattering processes along the lattice. Nevertheless, if the final set of scattering’s coincides, the resulting amplitudes $C_n$ are equal. The total number of paths for $a_{\nu,j'}$ is $N_{\nu,j'} = \sum_n f_n = \left(d(\sigma) - \delta_{\sigma}\right)$, which agrees with Eq. (3).

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$$a_{\nu,j'} = \exp[i\phi] \sum_{n=0}^{d(\sigma)} \left(\frac{r}{t}\right)^{2n+1} (-1)^n,$$
(a)-(b). Hence, a more balanced distribution among the states $j$’s is obtained. By the same token, the smooth (strong oscillatory) behavior for $|\Delta_j|$ small (large) is due to the fact that varying $j'$ in such interval will proportionally cause a small (large) change in the number of paths contributing to $a'_{j'}$. This results in a slow (rapid) variation of $a'_{j'}$ as function of $j'$.

Thus, the observed system fast spreading, e.g., in the unbiased case characterized by a linear dependence on $m$ for the standard deviation $<p_{j'} = |a_{j'}|^2 + |a_{j'}|^2$: $\Delta = \sqrt{\sum_{j'} (j'-j)^2 p_{j'} - \sum_{j'} (j'-j)p_{j'}^2} (\text{Fig. } \Delta \text{ (c))};$ due to (i)-(ii). In their turn, (i)-(ii) are a direct consequence of intricate interference effects among paths with different phases.

IV. CONCLUSION

Summarizing, our contribution here has been twofold. First, we propose a distinct approach – based on a true sum over paths history – to study QWs in general. It leads to some exact analytical results, which may be difficult to obtain by other means. Second, we properly quantify a fundamental characteristic of QWs, interference, explicit associating such phenomenon with the emergence of supperdiffusive behavior.

Hence, the present framework provides a powerful tool to test distinct aspects of QWs evolution, and whose complete comprehension is certainly an important step towards making QWs more reliable to distinct applications as in quantum computing.

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[38] $P_{s.p.} = W_{s.p.} \exp[iS_{s.p.}]$, with $S = m\gamma$ the action and $W$ the product of the corresponding coefficients gained by scattering off at the vertices along the way [31].

[39] For $k$ an integer, \binom{n}{k} is given by Maarten J. Kronenburg in arXiv:1105.3689v1 as: (i) for $n$ any nonnegative integer, $n!/(k!(n-k)!)$ if $0 \leq k \leq n$ and zero otherwise; (ii) for $n$ any negative integer, $(-1)^k \binom{-n+k-1}{k}$ if $k \geq 0$, $(-1)^{n-k} \binom{-n-k-1}{n-k}$ if $k \leq n$, and zero otherwise.

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