Nonclassicality of quantum walks

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We introduce a fidelity-based measure of nonclassicality $Q$ to quantify the differences between the dynamics of classical and quantum continuous-time walks over a graph. We provide universal, graph-independent, analytic expressions of $Q$, showing that at short times nonclassicality of quantum walks is due to the appearance of coherence, whereas for long times it depends only on the size of the graph, with quantumness contributing only partially to the overall nonclassicality. At intermediate times, nonclassicality does instead depend on the graph topology through its algebraic connectivity.

Classical and quantum walks provide powerful tools to describe the transport of charge, information or energy in several systems of interest for a wide spectrum of disciplines, ranging from quantum computing to biological physics [1-4]. In these contexts, in order to understand the very nature of the underlying dynamics, a question often arises on how to compare and assess the different behaviors of classical and quantum walks on a given structure. Quantum walks are also very useful to build quantum algorithms [5,8], and a comparison with the corresponding classical random walks is crucial to assess the possible quantum enhancement due to the faster spreading of probability distributions. As a consequence, the differences between classical and a quantum walk have been analyzed quite extensively, with short- and long-time behavior studied in both scenarios [9,13]. Signatures of the nonclassicality of the evolution involve the ballistic propagation of the quantum walker, compared to the classical diffusive analogue [14], and their measurement-induced disturbance or the presence of non-classical correlations, i.e. discord, in bipartite systems [15].

Continuous-time quantum walks (CTQWs) are usually introduced as the quantum generalization of continuous-time Markov chains, also called classical random walks (CRW). However, while the classical random walk is described through the evolution of a probability distribution, governed by a transition matrix (thus being an open system by construction), the CTQW dynamics is unitary with the Hamiltonian, given by the graph Laplacian, governing the evolution of the probability amplitudes [16]. Moreover, for regular lattices (i.e. graphs where each vertex has the same number of neighbors) the graph Laplacian is the discrete version of the continuous-space Laplacian thus it describes the evolution of a free particle on a discretized space [17]. On the contrary, for more general and complex graphs, the graph Laplacian cannot be straightforwardly associated to the classical Hamiltonian of a free particle.

Nonclassicality of QWs — Let us consider a finite undirected graph $G(V,E)$, where $V$ is the set of vertices and $E$ the set of edges. The state of the walker at a given time is described by the probability vector $\bar{p}(t) = e^{\nu L t} \bar{p}(0)$, where $\nu$ is the transition rate and $L$ is the transfer matrix, also known as the Laplacian of the graph [18], i.e. a symmetric matrix whose rows (or columns) sum to zero. In particular, $L_{jk} = 1$ (with $j \neq k$) if the nodes $j$ and $k$ are connected by an edge and $L_{jk} = 0$ if they are not. The diagonal elements of $L$ are given by $L_{jj} = -d_j$, where $d_j$ is the degree of node $j$, i.e. the number of edges connecting $j$ to other nodes. Given an initially localized probability distribution over the site $j$, and describing the system quantum mechanically, the evolution of a CRW may be described by the mixed state

$$E_c(\rho_j) = \sum_k p_{k,j}(t) |k\rangle \langle k|,$$

where $p_{k,j}(t) = \langle k | e^{\nu L t} | j \rangle$ is the transition probability from site $j$ to site $k$, $p_{k,j}(0) = \delta_{k,j}$, and the initial localized state is $\rho_j = |j\rangle \langle j|$. The orthonormal basis $\{|k\rangle\}_{k=1}^N$ describes states where the walker is localised on one of the $N$ sites of the graph. The completely-positive map $E_c$ describes the dynamics of the CRW. An initially localised quantum walker evolves instead unitarily, and the evolved state is given by the pure
where the coefficients \( \alpha_{kj}(t) = \langle j | e^{iLtt} | j \rangle \) represent the transition (tunneling) amplitudes between nodes \( j \) and \( k \) [10].

As it is apparent from Eqs. [1] and [2], the two evolutions lead to completely different final states. First of all, the classically evolved state of the CRW is always a mixed state, while for the CTQW we have a pure state at all times. In addition, quantum evolution admits superpositions of states and interference effects, which lead to dramatically different evolutions compared to the CRW. In turn, we remind that, while in classical case the Laplacian is just the transfer matrix of the Markov chain, for CTQW \( L \) is the effective Hamiltonian of the walker, i.e. \( H = -\nu L \). Hereafter, and without loss of generality (since it corresponds to fixing the time unit), we set the transition rate \( \nu = 1 \).

In order to quantify the differences between the classical and quantum dynamics of the walker, and to assess whether they may be ascribed to the appearance of genuine quantum features, we introduce a fidelity-based measure of nonclassicality (NC) for a quantum walker on a graph, and investigate its behavior in time. The nonclassicality \( Q(t) \) of a quantum walker on a graph \( G \) is given by

\[
Q(t) \equiv 1 - \min_{\rho_c} \mathcal{F}(\mathcal{E}_c(\rho_c), \mathcal{E}_q(\rho_c)),
\]

where \( \rho_c \) represents an initial classical state of the walker, i.e. a diagonal density matrix whose elements give the initial probability distribution over the graph \( G \). The quantity \( \mathcal{F}(\mathcal{E}_c(\rho_c), \mathcal{E}_q(\rho_c)) \) is the quantum fidelity between the quantum and the classical evolved state [12]:

\[
\mathcal{F}(\rho_1, \rho_2) = \left| \text{Tr} \sqrt{\rho_1 \rho_2 \sqrt{\rho_1 \rho_2}} \right|^2.
\]

Notice that in definition [3] we take the minimum of the fidelity over all initial classical states, in order to maximize the value of the NC. Let us now prove that for any graph the initial state that gives the minimum in Eq. [3] is a localized state, i.e. a state of the form \( \rho_j = |j\rangle \langle j| \).

**Theorem 1.** The initial classical state attaining the minimum in Eq. [3] is a localized state \( \rho_j = |j\rangle \langle j| \).

**Proof:** Let us consider a general classical state \( \rho_c = \sum_k z_k \rho_k \), with \( \rho_k = |k\rangle \langle k| \). The coefficients \( \{z_k\} \) give the initial probability distribution of the walker over the graph sites, satisfying the normalization condition \( \sum_k z_k = 1 \). In order to evaluate the NC of the system, we need to find the state \( \rho_c \) that minimizes the fidelity between the evolved CRW and the CTQW, described respectively by the quantum maps \( \mathcal{E}_c(\rho_c) \) and \( \mathcal{E}_q(\rho_c) \). The strong concavity property [20] applied to the square root of the fidelity gives:

\[
\sqrt{\mathcal{F}(\mathcal{E}_c(\rho_c), \mathcal{E}_q(\rho_c))} \geq \sum_k z_k \sqrt{\mathcal{F}(\mathcal{E}_c(\rho_k), \mathcal{E}_q(\rho_k))} = \sum_k z_k \mathcal{F}_k,
\]

where we introduced the fidelity between the classical and the quantum evolution of a particle initially localized on site \( k \): \( \mathcal{F}_k = \mathcal{F}(\mathcal{E}_c(\rho_k), \mathcal{E}_q(\rho_k)) \) and we omitted the explicit dependency on time. For regular graphs all nodes are equivalent and the fidelity does not depend on the initial site \( k \), hence \( F_k = F_0 \). Moreover thanks to the monotony of the square root function and the normalization condition, \( \mathcal{F}(\mathcal{E}_c(\rho_c), \mathcal{E}_q(\rho_c)) \geq F_0 \). The minimum is obtained for an initially localized state. For non-regular graphs, we have the same conclusion since the minimum of the convex combination of limited functions \( \sum_k z_k \mathcal{F}_k = \min_k \mathcal{F}_k \) and consequently the initial state attaining the minimum is localized.

**Universal properties of nonclassicality** — The NC is a positive quantity bounded between 0 and 1. Since we know from theorem [1] that the optimal initial state achieving the maximum of NC is a localized state \( \rho_j \), let us analyze the temporal behavior and properties of \( Q_j(t) = \sum_k \rho_{kj}(t) |\alpha_{kj}(t)|^2 \).

This expression allows us to explore the behavior of \( Q_j(t) = 1 - \mathcal{F}_j(t) \) for different time-regimes. In the short-time limit \( t \ll 1 \), we find that the nonclassicality depends only on the degree of the initial node \( d_j = \langle j | L | j \rangle \):

\[
Q_j(t \ll 1) = d_j.t.
\]

This result is obtained by expanding to first order the transition probability \( p_{kj}(t) \approx \delta_{kj} + t |\langle k | L | j \rangle| \) and the amplitude \( \alpha_{kj}(t) \approx \delta_{kj} + it |\langle k | L | j \rangle| \), with the reminder that the off-diagonal elements of \( L \) are positive, while the diagonal ones are negative. Therefore, the more the initial node is connected to the rest of the graph, the higher the nonclassicality of the evolution is. Since the classical probability tends to the flat distribution at large times \( \lim_{t \to \infty} p_{kj}(t) = \frac{1}{N} \), we can rewrite the fidelity in the long-time regime \( t \gg 1 \) as

\[
Q_j(t \gg 1) \approx 1 - \frac{1}{N}
\]

independently on the initial site \( j \) and the topology of the graph. The physical interpretation is clear: at short times what really matters is the connectivity of the initial node. This is a local phenomenon and does not depend on the dimension of the graph. As time passes, classical and quantum walker evolve, and explore the whole graph until the CRW achieves the stationary uniform distribution over the graph, while the CTQW periodically evolves both in populations and coherences. This leads to a stationary value for the NC, depending only on the size of the graph, which is a global property. This is illustrated in the left panel of Fig. [1] where we display, as an example, the behavior of the NC as a function of time for complete graphs of different sizes. The initial slope of the curves at short times is the vertex degree, while at long times the stationary value \( 1 - 1/N \) is reached. The intermediate-time behavior of the NC is related to the topology of the graph, with the main contribution coming from its algebraic connectivity. In order to see this, we notice that the squared amplitudes \( |\alpha_{kj}(t)|^2 \) are bounded (and oscillating) functions, whereas the classical transition probabilities may be written as \( p_{kj}(t) = \sum_{\lambda_s=1}^N e^{-|\lambda_s|^2 t} |\langle k | \lambda_s \rangle |^2 \). We have introduced the eigenvalues and eigenvectors of the Laplacian...
classically, taking into account the role of different initial positions. This is the average of the $Q_j(t)$ over the localized states, i.e. $\overline{Q}(t) = \frac{1}{N} \sum_{j=1}^{N} Q_j(t)$, which may be naturally referred to as the average nonclassicality. For regular graphs, it coincides with $Q(t)$, whereas for non-regular graphs it accounts for the fact that not all nodes lead to the same dynamics. The behaviour of $\overline{Q}(t)$ may be easily recovered from the previous analysis. We have $\overline{Q}(t \ll 1) \approx \bar{d} \alpha t$ for short times, where $\bar{d}$ is the average degree of the graph and $\overline{Q}(t \gg 1) \approx 1 - \frac{1}{N}$ for long times.

**The role of coherence and classical fidelity** — The nonclassicality quantifies how much the evolution of a quantum walker differs from the CRW counterpart. A question arises on whether this difference is due to the appearance of genuine quantum features, or it is just due to differences in the two maps $E_C$ and $E_Q$. As we will see the answer is not trivial and time dependent. Let us briefly recall the notion of coherence of a quantum state, a genuine quantum property with no classical analogue. Coherence may be properly quantified by the sum of the off-diagonal elements of the density matrix, i.e. $C(t) \equiv \sum_{k \neq j} |\rho_{kj}(t)|$. For the dynamics of a quantum walker the natural basis to consider is that of localized states. The coherence at time $t$ is thus given by $C_j(t) = (\sum_k |\alpha_{kj}(t)|^2)^{1/2}$, where the index $j$ refers to the localized initial state of the quantum walker. By construction, any classical state has zero coherence, i.e. it is incoherent. By expanding this expression for short times, up to first order, and comparing it with the expression of nonclassicality in Eq. 4 we find $Q_j(t) \quad \overset{t \ll 1}{\approx} \quad \frac{1}{2} C_j(t)$. It follows that the initial behavior of the nonclassicality at short times is governed solely by the amount of coherence created by the dynamics. In other words, the difference in the dynamics may be fully attributed to the appearance of genuine quantum features. On the other hand, this is no longer true at later time, where a substantial contribution to $Q(t)$ is due to differences in the distribution over sites. In order to prove this statement, let us introduce the classical fidelity between the probability distributions over the sites of CRW and CTQW, $F_j(t) = \sum_k \sqrt{p_{kj}(t)|\alpha_{kj}(t)|^2}$. For times large enough, we have $\sqrt{N} F_j(t) \approx \sum_k |\alpha_{kj}(t)|$ and, in turn, $N F_j^2(t) - C_j(t) \approx 1$. Putting together the above results, we may write

\begin{equation}
Q_j(t) = \begin{cases}
 Q_{JS}(t) = \frac{1}{2} C_j(t) & t \ll 1 \\
 Q_{JS}(t) = 1 - F_j^2(t) + \frac{1}{2} C_j(t) & t \gg 1
\end{cases}
\end{equation}

**Graph-dependent properties of nonclassicality** — The definition of NC involves a maximization over the initial state of the walker. There may be, however, situations where the $Q_j(t)$ themselves may be of interest: this is the case, for example, when we want to analyze the evolutions in similar topologies where the walker in initially localized in a specific site, i.e. we are not interested in performing the maximization. Such an example is illustrated in the central and right panels of Fig. 1 where we compare the behavior of the NC for the complete, star and wheel graphs. The central panel shows the quantity $Q_c(t)$ i.e. the NC evaluated for a dynamics starting from the central node $|c\rangle$, which is depicted in red for all graphs. However, if we compare the full nonclassicality $Q(t) = \max_{Q_j(t)}$ (see the right panel), we discover that $Q(t)$ for the wheel graph departs from the others in a certain time interval. $Q(t)$ increases linearly only at short times, according to Eq. \ref{eq:Q(t)} whereas, as time grows, the proportionality is lost and the topology of the graph plays a role in the behavior of the NC.

Let us now consider a different example, i.e. different graphs with size $N = 11$. We start with a ring graph, where all the nodes have degree equal to two. We then select one node, e.g. $|1\rangle$ and consider graphs with increasing number of links, i.e. we increase the node degree $d_1$ and show the nonclassicality $Q_1(t)$ in the left panel of Fig. 2. At short times, the ring graph shows the lowest value of $Q_1(t)$, but then it shows a maximum value in time, which is higher than the other graphs, i.e. the evolution of a quantum walker on a ring graph departs more from its classical counterpart compared to the other considered graphs.

Depending on the application at hand, one may also be interested in assessing the average dynamics over a graph. To this aim, let us also briefly discuss another measure of nonclassicality, taking into account the role of different initial positions. This is the average of the $Q_j(t)$ over the localized states, $\overline{Q}(t) = \frac{1}{N} \sum_{j=1}^{N} Q_j(t)$, which may be naturally referred to as the average nonclassicality. For regular graphs, it coincides with $Q(t)$, whereas for non-regular graphs it accounts for the fact that not all nodes lead to the same dynamics. The behaviour of $\overline{Q}(t)$ may be easily recovered from the previous analysis. We have $\overline{Q}(t \ll 1) \approx \bar{d} \alpha t$ for short times, where $\bar{d}$ is the average degree of the graph and $\overline{Q}(t \gg 1) \approx 1 - \frac{1}{N}$ for long times.

![Figure 1](image-url) Left: nonclassicality $Q(t)$ for the complete graph for different values of $N$. Center: nonclassicality $Q_c(t)$ for the complete, star and wheel graphs, starting from the initial central site $|c\rangle$, depicted in red. Right: nonclassicality $Q(t)$ for the same graphs.
Eq. (6) shows that that for short times nonclassicality of quantum walks is due to the appearance of coherence, whereas for long times quantum features accounts only partially for the difference between the two dynamics. In this regime, nonclassicality is the sum of the normalised coherence and the difference between the probability distributions over the graph. We also remark that $Q$ no longer depends on the topology of the consider graph, but rather only on its size. In order to assess the generality of this statement, and the range of validity Eq. (6), we have considered different classes of graphs and evaluated the ratios $\gamma_K(t) = Q(t)/Q_K(t)$, $K = S, L$ between the exact nonclassicality (calculated numerically) and its limiting expressions in Eq. (6) for short and long times. In the central panel of Fig. 2 we report the two values of $\gamma$ for a set of graphs of size $N = 11$. As it is apparent from the plot, the range of validity of the short time expression $Q_S(t)$ depends quite strongly on the kind of graph, whereas the convergence to the asymptotic value $Q_L(\infty) = 1 - 1/N$ is almost independent on the graph, and it is achieved quite rapidly. The same rapid convergence $\delta(t) \to 1/N$ may be seen in the difference $\delta(t) = F^2(t) - C(t)/N$ between the square of the classical fidelity and the size-normalized coherence. Here the convergence time increases with the size of the graph, still being independent on its topology.

Discussion and conclusions — We have introduced a fidelity-based measure of nonclassicality to properly compare classical and quantum walks over a graph, also discussing the role of size and topology of the graph. Our results show that at short times, nonclassicality of quantum walks is proportional to local connectivity, and in turn to coherence, i.e. to the appearance of a genuine quantum feature. On the other hand, in the long time limit, quantumness plays only a partial role, since nonclassicality is the sum of a size-normalised measure of coherence and the classical distance between the probability distributions over the graph. The graph topology is not relevant in those two limiting regimes, whereas it plays a role in determining the nonclassicality at intermediate times. Notice that the two terms in $Q_L(t)$ are approximately of the same magnitude, i.e. coherence and classical distance contribute almost equally to the nonclassicality.

From the physical point of view, the behavior of $Q(t)$ tells us that the difference between CRW and CTQW may be initially acribed to the ability of a quantum walker to tunnel between sites, whereas for longer times coherence cannot fully account for the difference in the dynamics. In this regime, nonclassicality is also due to the periodic nature of CTQW dynamics, compared to the diffusive one of CRW, which leads to an equilibrium state. In other words, the differences in the long times dynamics should be equally acribed to the appearance of quantum features, as well as to the different nature (open vs closed system) of the two dynamical models. We expect our measure to represent a tool in assessing the role of quantum features in the dynamics of quantum complex networks. We also believe that it paves the way to define the nature and the amount of nonclassicality in many particle quantum walks.

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