Degree Distribution in Quantum Walks on Complex Networks

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We relate the average long time probability of finding a quantum walker at a node to that for a corresponding classical walk. The latter is proportional to the node degree. We replace the state dependence of quantum evolution by a partial order, bounding the quantumness of the walker in terms of the energy of the initial state and the spectral gap of the complex network. For a uniform initial state, we identify complex network classes and regimes for which the classical degree-dependent result is recovered and others for which quantum effects dominate. The importance of quantum effects, or the quantumness of a complex network, is given by the Rényi entropy of order 1/2 of the normalized weighted degrees, which can be upper bounded by the Shannon entropy.

I. INTRODUCTION

The distribution of degrees in a network links phenomena observed in an assortment of physical systems [1–5], ranging from the Internet [6, 7] to social or ecological networks [8–10]. Here we take the degree (called strength by some) of a node to be the centrality measure given by the sum of the weighted and undirected connections to its neighbors. The degree distribution gives the frequency with which nodes take degree values. A well known example of the importance of degree distribution in physical processes stems from the steady state of a classical stochastic walk, where the long time probability of finding a walker at each node is proportional to the degree of that node [4]. Here we show that the degree distribution appearing in classical walks also plays a central role in the unitary quantum walks.

By doing so, we build on the traditional theory of complex networks, which, through a growing number of recent works has been applied in various ways within quantum mechanics, including [11–18]. In particular, quantum walks have been considered on complex networks [11–13, 17–21]. Quantum walks are a powerful tool to simulate and study transport properties on quantum systems [22–24] and date as far back as Feynman [25, 26]. Moreover, the unitary dynamics of any discrete quantum system can be re-expressed and interpreted as a single-particle quantum walk.

In this work we study the long time average probability of finding a walker at a node during a continuous-time unitary quantum walk. In doing so we overcome the first challenge to analyzing unitary quantum walks, as opposed to some open quantum walks (see e.g. [27, 28]), which is the lack of a long time stationary state. We find that for a walker with zero energy the long time average probability distribution for a wide class of quantum walks is equal to that of a corresponding classical walk. This is related to the node degrees. The energy of the walker upper bounds the difference between the quantum and classical distributions—what we call the network quantumness of the walk. By giving partial order to the states of the walk in terms of energy, we overcome the second challenge of understanding unitary quantum walks, which is the dependence on the initial state.

Figure 1. Relating stochastic and quantum walks. An undirected weighted network (graph) $G$ is represented by a symmetric, off-diagonal and non-negative adjacency matrix $A$. There is a projection sending $A$ (by summing columns) to diagonal $D$ with entries given by the weighted degree of the corresponding node. The node degrees are proportional to the steady state probability distribution of the continuous-time stochastic walk (with uniform escape rate from each node) generated by $H_G = D^{-1}$, where $L = D - A$ is the Laplacian. The steady state probabilities, represented by the vector $|\pi_0\rangle$, are proportional to the node degrees. We generate a corresponding continuous-time unitary quantum walk by the Hermitian operator $H_Q = D^{-1/2}L D^{-1/2}$, which is similar to $H_G$. The probability of being in a node in the stochastic stationary state $|\pi_0\rangle$ and the probability arising from the quantum ground state are respectively equal and proportional to the node degree.
As an example, we both analytically and numerically study the walk resulting from an evenly distributed initial state. We find an additional connection to degree for this case, namely that the quantumness of the walk is itself controlled by the heterogeneity of the degrees, which we quantify in terms of Rényi entropy. These results are confirmed numerically for a range of complex network structures, including the Barabási-Albert (BA), Erdős-Rényi (ER), Watt-Strogatz (WS) and random geometric (RG) networks, providing further insight into the interplay between network topology and the observed average quantum effects. The numerics enable us to view the form of the quantum deviations to the zero energy/classical result. We find that in general they increase the probability of finding the walker at nodes with a small degree.

In Sec. II we formulate and study the problem analytically, first for a stochastic walk and then for a quantum walk. Following this, in Sec. III we confirm our analytical results for the quantumness of a quantum walk numerically and explore the way in which the quantum long time average deviates from the corresponding classical distribution. We conclude with a discussion in Sec. IV.

II. WALKS FRAMEWORK

We consider a walker moving on a connected network of $N$ nodes, with each weighted undirected edge between nodes $i$ and $j$ described by the element $A_{ij}$ of the off-diagonal adjacency matrix $A$. The matrix is symmetric ($A_{ij} = A_{ji}$) and has real, non-negative entries. We use Dirac notation and represent $A = \sum_{ij} A_{ij} |i⟩⟨j|$ in terms of $N$ orthonormal vectors $|i⟩$.

The network gives rise to both a quantum walk and a corresponding classical walk. The classical stochastic walk $S(t) = e^{-H_C t}$ is generated by the infinitesimal stochastic (see e.g. Refs. [29–31]) operator $H_C = LD^{-1}$, where $L = D - A$ is the Laplacian and $D = \sum_i d_i |i⟩⟨i|$ is defined by its diagonal elements, the degrees, $d_i = \sum_j A_{ij}$. For this classical walk, the total rate of leaving each node is identical. The corresponding unitary quantum walk $U(t) = e^{-iH_Q t}$ is generated by the Hermitian operator $H_Q = D^{-1/2}L D^{-1/2}$. For this quantum walk, the overlaps $⟨i | H_Q | j⟩$ at each node is identical. The generators $H_C$ and $H_Q$ are similar matrices, related by $H_Q = D^{-1/2}H_C D^{1/2}$. This mathematical framework, represented in Fig. 1, underpins our analysis.

As we will describe in Sec. II.A, the long time behavior of the classical walk generated by $H_C$ has been well explained in terms of its underlying network properties, specifically the degrees $d_i$. Our goal in Sec. II.B is to determine the role this concept plays in the quantum walk generated by $H_Q$.

A. Classical Walks

In the classical walk the probability $P_i(t)$ of being at node $i$ at time $t$ is $|P_i(t)| = S(t)|P_0⟩$, where $|P(t)| = \sum_i P_i(t)|i⟩$. The stationary states of the walk are described by eigenvectors $|\pi^c_i⟩$ of $H_C$ with eigenvalues $\lambda_i$ equal to zero. We assume throughout this work that the walk is connected, i.e., it is possible to transition from any node to any other node through some series of allowed transitions. In this case there is a unique eigenvector $|\pi_0⟩ = |P_0⟩$ with $\lambda_0 = 0$, and $\lambda_i > 0$ for all $i \neq 0$[32]. This (normalized) eigenvector $|P_0⟩ = \sum_i (C)v_i|i⟩$ describes the steady state distribution

$$⟨P_0⟩ = \sum_i \frac{d_i}{\sum_j d_j}. \tag{1}$$

In other words, the process is ergodic and after long times the probability of finding the walker at any node $i$ is given purely by the importance of the degree $d_i$ of that node in the network underlying the process.

B. Quantum Walks

When considering quantum walks on networks, it is natural to ask what is the long time behavior of a quantum walker [11, 12, 33, 34]. The unitary evolution will not drive the system towards a steady state. Therefore, to obtain a static picture we consider the long time average distribution of $|P_0⟩$, which reads

$$⟨P_0⟩ = \lim_{T \to \infty} \frac{1}{T} \int_0^T dt |⟨i|U(t)|\Psi(0)⟩|^2. \tag{2}$$

For ease of comparison with $|P_0⟩$ we will also write the distribution in Eq. (3) as a ket $|P_Q⟩ = \sum_i ⟨i|P(t)|i⟩$. Unlike the classical case, Eq. (2) depends on the initial state $|\Psi(0)⟩$.

Interference between subspaces of different energy vanish in the long time average so we obtain an expression for the probability $⟨P_Q⟩_i$ in terms of the energy eigenspace projectors $\Pi_j$ of the Hamiltonian $H_Q$,

$$⟨P_Q⟩_i = \sum_j |⟨i|\Pi_j|\Psi(0)⟩|^2. \tag{3}$$

Here $\Pi_j = \sum_k |\phi_{jk}⟩⟨\phi_{jk}|$ projects onto the subspace spanned by the eigenvalues $|\phi_{jk}⟩$ of $H_Q$ corresponding to the same eigenvalue $\lambda_j$. In other words, the long time average distribution is a mixture of the distribution arising from each eigenspace, with the weights given by the overlap of the initial state with the eigenspaces.

Due to the similarity transformation $H_Q = D^{-1/2}H_C D^{1/2}$ the classical $H_C$ and quantum $H_Q$ generators share the same eigenvalues $\lambda_i \geq 0$, and have eigenvectors related by $|\phi_{ik}⟩ = D^{-1/2}|\pi^c_i⟩$ up to their normalizations. In particular, the unique eigenvectors corresponding to $\lambda_0 = 0$ are $|\pi_0⟩ = D|1⟩$ and $|\phi_0⟩ = D^{1/2}|1⟩$. 

up to their normalizations, with $|1\rangle = \sum_i |i\rangle$. Therefore the probability vector describing the outcomes of a measurement of the quantum ground state eigenvector $|\phi_0\rangle$ in the node basis is the classical steady state distribution $|\pi_0\rangle = |P_C\rangle$.

The state vector $|P_C\rangle$ appears in Eq. (3) for the quantum long time average distribution $|P_Q\rangle$ with weight $|\langle \phi_0 | \Psi(0) \rangle|^2$. Accordingly we split the sum in Eq. (3) into two parts, the first we call the “classical term” $|P_C\rangle$ and the rest we call the “quantum correction” $|\tilde{P}_Q\rangle$, as

\[ |P_Q\rangle = (1 - \varepsilon)|P_C\rangle + \varepsilon|\tilde{P}_Q\rangle. \tag{4} \]

The normalized quantum correction $|\tilde{P}_Q\rangle = \sum_i (\tilde{P}_Q)_i |i\rangle$ is given by

\[ (\tilde{P}_Q)_i = \frac{1}{\varepsilon} \sum_{j \neq 0} |\langle i | \Pi_j | \Psi(0) \rangle|^2, \tag{5} \]

and the weight

\[ \varepsilon = 1 - |\langle \phi_0 | \Psi(0) \rangle|^2, \tag{6} \]

we call quantumness is a function both of the complex network topology and the initial state.

We can think of the parameter $\varepsilon$, which controls the classical-quantum mixture, as the quantumness of $|P_Q\rangle$ for the following three reasons. First, the proportion of the elements in $|P_Q\rangle$, that corresponds to the quantum correction is $\varepsilon$. Second, the trace distance between the normalized distribution $(P_C)_i$ and the unnormalized distribution $(1 - \varepsilon)(P_C)_i$ forming the classical part of the quantum result is also $\varepsilon$. Last, using a triangle inequality, the trace distance between the normalized distributions $(P_C)_i$ and $(P_Q)_i$ is upper bounded by $2\varepsilon$.

This expression for the quantumness in Eq. (6) enables us to make some physical statements about a general (even mixed) initial state. By realizing that $|\phi_0\rangle$ is the ground state and assuming a gap $\Delta$ in the energy spectrum $\Delta = \min_{\lambda_i \neq 0} \lambda_i$, the above implies a bound $E \geq \varepsilon \Delta$ for the quantumness $\varepsilon$ of the walk in terms of the energy $E = \langle H_Q \rangle$ of the system. We see that the classical stationary probability distribution will be recovered for low energies. This result provides a partial order bounding the quantumness of walker states in terms of the equivalence class of states sharing the same energy.

C. Degree Distribution and Quantumness

Quantumness is both a function of the network adjacency matrix and the initial state. To compare the quantumness of different complex networks, we fix the initial state $|\Psi(0)\rangle$. For our example we choose the even superposition state $|\Psi(0)\rangle = |1\rangle/\sqrt{N}$. This state has several appealing properties, for example, it is invariant under node permutations and independent of the arrangement of the network.
In this case the quantumness is given by the expression

\[ \varepsilon = 1 - \frac{1}{N} \exp \left( -H_{1/2} \left( \left\{ \frac{d_i}{\sum_j d_j} \right\} \right) \right) , \]

(7)

where \( \langle d \rangle = \frac{\sum_i d_i}{N} \) is the average degree and \( \langle \sqrt{d} \rangle = \sum_i \sqrt{d_i}/N \) is the average root degree of the nodes. As such, the quantumness depends only on the degree distribution of the network and increases with network heterogeneity.

This statement is quantified by writing the quantumness

\[ \varepsilon = 1 - \frac{1}{N} \exp \left[ H_{1/2} \left( \left\{ \frac{d_i}{\sum_j d_j} \right\} \right) \right] , \]

in terms of the Rényi entropy

\[ H_q(p_i) = \frac{1}{1-q} \ln \left( \sum_i p_i^q \right) , \]

(9)

where \( d_i/\sum_j d_j = (P_C)_i \) are the normalized degrees.

To obtain an expression in terms of the (perhaps) more familiar Shannon entropy \( H_1 \) (obtained by taking the \( q \to 1 \) limit of Eq. (9)), we recall that the Rényi entropy is non-increasing with \( q \) [35]. This leads to the upper bound

\[ \varepsilon \leq 1 - \frac{1}{N} \exp \left[ H_1 \left( \left\{ \frac{d_i}{\sum_j d_j} \right\} \right) \right] , \]

(10)

The quantumness approaches this upper bound in the limit that \( M \) nodes have uniform degree \( d_i = M\langle d \rangle/N \) and all others have \( d_i = 0 \). This limit is never achieved unless \( M = N \) and \( \varepsilon = 0 \), e.g., a regular network.

In another limit, the quantumness takes its maximum value \( \varepsilon = (N-2)/N \approx 1 \) when the degrees of two nodes are equal and much larger than those of the others (note that the symmetry of \( A \) prevents the degree of a single node from dominating). In the case that \( A_{ij} \in \{0,1\} \), i.e., the network underlying the walks is not weighted, the quantumness of a connected network is more restricted. It is maximized by a walk based on a star network—where a single node is connected to all others. For a walk of this type \( \varepsilon = 1/2 - \sqrt{N-1}/N \approx 1/2 \).

Next Sec. III we confirm the above analytical findings numerically and at the same time numerically study the form of the quantum correction \( |P_Q| \) given by Eq. (5) for a range of complex network types.

**III. NUMERICAL RESULTS**

We consider walkers on general classes of networks, each with a fundamentally different complex network topology. To start, we consider non-weighted binary networks \( A_{ij} \in \{0,1\} \) with \( N = 500 \) nodes and average degree \( \langle d \rangle \approx 6 \). If a disconnected network is obtained, only the giant component is considered. Specifically we consider the BA scale free network [1], the ER [36] and the WS [37] small world networks, and the RG (on a square) [38], a network without the scale free or small world characteristics.

The long time average probability of being on each node \( i \) is plotted against its degree \( d_i \) for a quantum (\( P_Q \)) and stochastic (\( P_C \)) walk in Fig. 2. The two cases are nearly identical for these binary networks and the evenly distributed initial state, illustrating that the quantumness \( \varepsilon \) is small. We have in fact calculated the quantumness directly for each network type, yielding \( \varepsilon = 0.130, 0.043, 0.016, 0.040 \) for the BA, ER, WS and RG networks, respectively. Within these, the BA network shows the highest quantum correction. This is expected since the BA network has the higher degree heterogeneity. The WS network, which is well known to have quite uniform degrees [39], is accordingly the network with the lowest quantum correction.

For many of the network types the typical quantumness can be obtained from the expected (thermodynamic limit) degree distribution. In the BA network, the degree distribution approximately obeys the continuous probability density \( P(d) \approx \langle d \rangle^d e^{-\langle d \rangle}/d! \) [1]. Integrating this to find the moments, results in \( \varepsilon = 1/9 \), which is independent of the average degree \( \langle d \rangle \) and is compatible with our numerics. The degree distributions of the ER and RG networks both approximately follow the Poissonian distribution \( P(d) \approx \langle d \rangle^d e^{-\langle d \rangle}/d! \) for large networks, which explains the similarity of their quantumness \( \varepsilon \) values. For \( \langle d \rangle = 6 \) we recover \( \varepsilon \approx 0.046 \), which is compatible with the values for the particular networks we generated. From the general form, calculating the quantumness numerically and performing a best fit we find

![Figure 3. (Color online) Quantumness and degree entropy. The value of \( \varepsilon \) against \( H_1 \) (Eq. (9)) for the four different networks considered in Fig. 2 as well as random regular (RR) (a network with the same degree for each node, in this case we consider a 6-regular network) and star (ST) networks (black +). We also plot \( \varepsilon \) and \( H_1 \) for the BA network in the case that the internode weights are randomly varied using \( M \) iterations, for increasing \( M \) (bottom to top, gray to orange \( \times \)). The quantumness \( \varepsilon \) increases and entropy \( H_1 \) decreases with \( M \). The red dashed line represents the upper bound of Eq. (10).](image-url)
that \( \varepsilon \approx \kappa_1 \langle d \rangle^{-\kappa_2} \), with fitting parameters \( \kappa_1 = 0.429 \) and \( \kappa_2 = 1.210 \).

The size of the quantum effects can be enhanced by introducing heterogeneous weights \( A_{ij} \) within a network. We have done this for a BA network using \( M \) iterations of the following procedure. A pair of connected nodes is randomly selected then the associated weight is doubled or halved at random. As anticipated, large \( M \) implies a large discrepancy between the classical and quantum dependence of the long time average probability on degree was found, illustrated in Fig. 2. As \( M \) is increased, the quantumness approaches the bound given in Eq. (10), as shown in Fig. 3. In fact, most networks are found close to saturating this bound, especially for low quantumness.

Finally, our numerical calculations reveal the behavior of the quantum part \( \tilde{P}_Q \) of the long time average node occupation. We find that the quantum part enhances the long time average probability of being at nodes with small degree relative to the classical part. More precisely \( \langle \tilde{P}_Q \rangle_i / \langle P_C \rangle_i \) exhibits roughly \( \langle d_i \rangle^{-\kappa_3} \) scaling, with \( \kappa_3 \approx 1 \), as shown in Fig. 4. Interestingly, there is a correlation between the amount of enhancement, given by \( \kappa_3 \), and the type of complex network. The network types with smaller diameters (order of increasing diameter: BA, then ER and WS, then RG) have the smallest \( \kappa_3 \), and the quantum parts enhance the low degree nodes least. Moreover, the enhancement \( \kappa_3 \) seems to be quite independent of the internode weights. Thus our numerics show a qualitatively common quantum effect for a range of complex network types. Quantitative details vary between the network types, but appear robust within each type.

**IV. DISCUSSION**

We have studied both analytically and numerically the average long time probability distribution for the location of a quantum walker on a complex network. Specifically we compared this to the analogous result for a classical walker, in which the probability distribution is given by the normalized degrees. We showed that the classical result emerges from the quantum dynamics for low energies. In particular, for the evenly distributed initial state the size of the difference between the two (the quantumness) depends only on the degrees. This shows that degree distribution can be as important and illuminating in quantum walks as in their classical counterparts, and guides us to regimes in which quantum effects are more or less prominent. Our numerics show that for a remarkably diverse types of network the quantum effects are qualitatively similar; they acted to reduce the degree dependence of the average probability of a walker being on a node.

[1] A.-L. Barabási and R. Albert, Science 286, 509 (1999).
[2] R. Albert and A.-L. Barabási, Rev. Mod. Phys. 74, 47 (2002).
[3] M. E. J. Newman, SIAM Review 45, 167 (2003).
[4] M. Newman, Networks: An Introduction (Oxford University Press, Inc., New York, NY, USA, 2010).
[5] D. J. de Solla Price, Science 149, 510 (1965).
[6] M. Faloutsos, P. Faloutsos, and C. Faloutsos, SIGCOMM Comput. Commun. Rev. 29, 251 (1999).
[7] R. Albert, H. Jeong, and A. Barabási, Nature 401, 130 (1999).
[8] S. Wasserman and K. Faust, Social Network Analysis. Methods and Applications (Cambridge University Press, 1994).
[9] D. J. Watts, P. S. Dodds, and M. E. J. Newman, Science 296, 1302 (2002).
[10] M. E. J. Newman, Phys. Rev. E 66, 016128 (2002).
[11] O. Müllken and A. Blumen, Phys. Rep. 502, 37 (2011).
[12] E. Sánchez-Burillo, J. Duch, J. Gómez-Gardeñes, and D. Zueco, Nat. Sci. Rep. 2, 605 (2012), 10.1038/srep00605.
[13] D. J. Watts, P. S. Dodds, and M. E. J. Newman, Science 296, 1302 (2002).
[14] M. E. J. Newman, Phys. Rev. E 66, 016128 (2002).
[15] O. Müllken and A. Blumen, Phys. Rep. 502, 37 (2011).
[16] E. Sánchez-Burillo, J. Duch, J. Gómez-Gardeñes, and D. Zueco, Nat. Sci. Rep. 2, 605 (2012), 10.1038/srep00605.
[17] G. D. Paparo and M. A. Martin-Delgado, Sci. Rep. 2, 444 (2012).
[18] M. Cuquet and J. Calsamiglia, Phys. Rev. Lett. 103, 240503 (2009).
[19] S. Pereseguers, M. Lewenstein, A. Acín, and J. Cirac, Nature Physics 6, 539 (2010).
[20] S. Pereseguers, D. Cavalcanti, G. J. Lapeyre, M. Lewenstein, and A. Acín, Phys. Rev. A 81, 032327 (2010).
[21] S. Pereseguers, P. Zanardi, and D. A. Lidar, Phys. Rev. Lett. 108, 230506 (2012).
[22] Z. Zimboras, M. Faccin, Z. Kadar, J. Whitfield, B. Lanyon, and J. Biamonte, “Quantum transport enhancement by time-reversal symmetry breaking,” (2012), arXiv:1303.2074.
[23] J. Kempe, Contemp. Phys. 44, 307 (2003).
[24] P. E. Venegas-Andraca, Synthesis Lectures on Quantum Computing 1, 1 (2008).
[25] S. Garnerone, Phys. Rev. A 86, 032342 (2012).
[26] E. Farhi and S. Gutmann, Phys. Rev. A 58, 915 (1998).
[27] F. Caruso, A. W. Chin, A. Datta, S. F. Huelga, and M. B. Plenio, The Journal of Chemical Physics 131, 105106 (2009).
[28] M. Mohseni, P. Rebentrost, S. Lloyd, and A. Aspuru-Guzik, J. Chem. Phys. 129, 174106 (2008).
[29] R. P. Feynman, R. B. Leighton, and M. Sands, The Feynman Lectures on Physics, 2nd ed. (Addison Wesley, 2005).
[30] D. J. Watts and S. H. Strogatz, Nature 393, 409 (1998).
[31] M. Penrose, Random Geometric Graphs, Vol. 5 (Oxford University Press on Demand, 2003).
[32] A. Barrat and M. Weigt, The European Physical Journal B 13, 47 (2000).

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