Information Dimension of Dissipative Quantum Walks

P. Schijve† and O. Mülken‡

Physikalisches Institut, Universität Freiburg, Hermann-Herder-Strasse 3, 79104 Freiburg, Germany

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We study the temporal growth of the von Neumann entropy for dissipative quantum walks on networks. By using a phenomenological quantum master equation, the quantum stochastic walk (QSW), we are able to parametrically scan the crossover from purely coherent quantum walks to purely diffusive random walks. In the latter limit the entropy shows a logarithmic growth, which is proportional to the information dimension of the random walk on the network. Here we present results for the von Neumann entropy based on the reduced density operator of the QSW. It shows a similar logarithmic growth for a wide range of parameter values and networks. As a consequence, we propose the logarithmic growth rate of the von Neumann entropy to be a natural extension of the information dimension to dissipative quantum systems. We corroborate our results by comparing to numerically exact simulations.

Much effort has been put into understanding dynamical properties of excitation transfer on various networks [1]. Based on the continuous-time quantum walk (CTQW) [2], one of the intriguing questions is if it is possible to achieve a classification of its quantum dynamics, similar to the classical universality classes [3]. For continuous-time random walks (CTRW), this can be done by studying the scaling exponents of dynamical properties such as the mean square displacement, the mean first passage time and the average return probability [4, 5]. Due to the highly oscillatory nature of the CTQW how- ever, many of these exponents do not translate well to the quantum regime [1]. In this letter, we show that this problem can be approached by studying the so-called information dimension associated with a CTQW on a network in a dissipative environment.

For classical random walks on networks, the information dimension is a dynamical exponent which is defined by the logarithmic growth of the entropy [6, 7]. Recently, much interest has been shown in the growth of the (entanglement) entropy in diffusive and disordered systems [8–10]. Additionally, much attention has recently been given to understand the entropy production rate in open quantum systems [11, 12]. In this letter, we provide a new perspective on the entropy growth of dissipative quantum systems [11–16]. In order to model the incoherent hopping, i.e., a CTRW between the nodes of the network after most coher- ent signatures are gone [13]. In order to model the CTRW, we utilize the freedom of choosing the set of Lindblad operators $L_{kl}$ [13]: It can be shown that the Lindblad operator $L_{nn} = |m \rangle \langle n |$, for $m \neq n$, models an incoherent transition from node $| n \rangle$ to node $| m \rangle$ [14–16]. Following Förster theory or Marcus’ theory of electron transport, we can then estimate the incoherent transition rates $k_{n \rightarrow m}$ between the nodes $| n \rangle$ and $| m \rangle$ by using Fermi’s golden rule, i.e., $k_{n \rightarrow m} \sim | \langle m | H_0 | n \rangle |^2$ [15, 16]. Upon setting $\lambda_{mn} = k_{n \rightarrow m}$ we obtain the correct CTRW from the dissipator.

We now use the Lindblad equation to construct a pheno- menological model that allows us to interpolate between these two limiting scenarios. This model is also known as the Quantum Stochastic Walk (QSW) [14]. The master equation then takes the following form:

$$\frac{d \rho_{\alpha}(t)}{dt} = (1 - \alpha) L_{\text{CTQW}}[\rho_{\alpha}(t)] + \alpha (L_{\text{CTRW}}[\rho_{\alpha}(t)] + L_{\text{deph}}[\rho_{\alpha}(t)])$$

with $\alpha \in [0, 1]$. $L_{\text{CTQW}}[\rho_{\alpha}(t)] = -i [H_0, \rho_{\alpha}(t)]$. Furthermore, $L_{\text{CTRW}}[\rho_{\alpha}(t)]$ models that part of the dissipator in Eq. (2) which describes the environmentally induced
a CTRW, while $L_{\text{depth}}[\rho_\alpha(t)]$ is that part of the dissipator which induces a localized dephasing process. To model the latter, we choose the (diagonal) Lindblad operators $L_{\text{onm}} = |m\rangle \langle m|$ and, for simplicity, we choose the dephasing rates to be $\lambda_{\text{on}} \equiv \lambda = 1$.

In order to validate our model for more realistic systems, we also use the numerically exact Hierarchy Equations of Motion approach (HEOM) to solve the reduced dynamics on the underlying network. The latter is reflected in the scaling behaviour of the probability to return or to remain at the origin, $I_{\alpha} = -\lim_{t \to \infty} S_{\alpha}(t,\tau)$, which increases from $S_{\alpha}(0,\alpha) = 0$ to its maximal value $\ln N$ for all $\alpha > 0$. Here, we are interested in the question if the growth of $S_{\alpha}(t,\alpha)$ can be related to certain scaling exponents associated with the dynamics on the underlying network.

In the classical limit, $(\alpha \to 1)$ $S_{\alpha}(t,\alpha)$ reduces to the classical Shannon entropy $H(t)$ of the environmentally induced CTRW:

$$H(t) \equiv \lim_{\alpha \to 1} S_{\alpha}(t,\alpha) = -\sum_k p_{kj}(t) \ln[p_{kj}(t)],$$

where $p_{kj}(t) = \lim_{\alpha \to 1} \langle k|\rho_\alpha(t)|j\rangle$, given that $\rho_\alpha(0) = |j\rangle \langle j|$. For various networks, it has been numerically shown that $H(t)$ grows linearly with $\ln(t)$ after an initial/transient time $t_1$. The logarithmic growth rate is now defined as the CTRW variant of the information dimension, i.e., $H(t) \sim d_1 \ln t$. We pause to note that this definition is akin to the definition of the information dimension of chaotic systems. For a discrete-time random walk, having performed $M$ steps, it is defined as $d_1 = I_M/\ln M$. Here $I_M = -\sum_{k=1}^M P_k \ln P_k$, with $P_k$ being the probability of visiting the $k$-th site. Upon taking the limit to the CTRW, this matches our definition.

The existence of a logarithmic growth for CTRW can be shown analytically by assuming that the propagator for the CTRW on a generic complex network can be formulated as a stretched exponential, $p_{kj}(t) \sim t^{-d_j/2} \exp(-(a\xi_k^t)^t)$, where $\xi_k = r_k t^{-d_j/2d_f}$. Here, $r_k$ is the position of the $k$-th node relative to node $j$, $d_f$ the fractal dimension and $d_s$ the spectral dimension of the network. The latter is reflected in the scaling behaviour of the probability to return or to remain at the origin, i.e., $p_{jj}(t) \sim t^{-d_s/2}$. Substituting this form into the definition of $H(t)$ results in:

$$H(t) = \frac{d_s}{2} \ln t + t^{-d_s/2d_f} \sum_k r_k^t p_{kj}(t) \approx \frac{d_s}{2} \ln t. \quad (6)$$

In this case we thus obtain $d_1 = d_s/2$.

Since the von Neumann entropy is well-defined for all values of $\alpha$ and contains the Shannon entropy $H(t)$ as a limiting case, we now introduce the (possibly $\alpha$-dependent) information dimension $d_1(\alpha)$ for the QSW in a similar way as above. Provided that $S_{\alpha}(t,\alpha)$ grows linearly with $\ln(t)$ for intermediate times, $\alpha t$ is defined by:

$$S_{\alpha}(t,\alpha) \sim \alpha t (\ln(t)) \quad (7)$$

Note that for $\alpha = 0$, the system is always in a pure state, resulting in $S_{\alpha}(t,\alpha = 0) = 0$ for all $t$. Therefore it is not possible to define $d_1(\alpha)$ for $\alpha = 0$ in this way.

Since an analytic solution of Eq. (3) is only possible for a few cases and for small systems we proceed with a numerical analysis of two important examples. As prototypes for opposing dynamical behaviors we take the linear chain and the so-called Sierpinski gasket. For the former, the CTQW is more efficient, i.e. faster than the corresponding CTRW, while for the latter the converse is true. The Sierpinski gasket is a deterministic fractal structure where each new generation $g$ is determined by subdividing each triangle into three new sub-triangles such that the number of nodes in generation $g$ is given by $N_g = 3(3^g - 1)/2$. Fig. 4 shows the von Neumann entropy as a function of time (in log-lin scale) for different values of $\alpha$ for (a) a line of $N = 100$ nodes and for (b) a Sierpinski gasket of generation $g = 5$ with $N = 123$ nodes. The first thing to notice is that at a given small (transient) time ($t < 1$) the entropy in the CTQW limit is smaller than in the CTRW limit. In order to understand this, we consider a dimer, i.e. a network of only two nodes. It is straightforward to show that for times $t \ll 1$ one obtains $S_{\alpha}(t,\alpha) \approx at - \ln(\alpha t)$. A similar result has also been obtained for a slightly different model in Ref. [27].

However, with increasing time, the increase in entropy becomes larger the smaller the value of $\alpha$. Before the entropy reaches its stationary value, we find the logarithmic scaling for both the line and the Sierpinski gasket. While the scaling region stretches over a rather long period of time for values of $\alpha \geq 0.2$, namely $t \in [10, 100]$ for the line and $t \in [1, 10]$ for the gasket, this region is smaller the smaller the value of $\alpha$. For $\alpha = 0.1$ and for the finite structures considered here, the scaling regions become very small. We are certain that this issue can be resolved by computing the entropy for a larger chain in order to delay the approach to the equilibrium state. The difference in the time scales for the line and the Sierpinski gasket can be understood when realizing that the
Sierpinski gasket of generation $g=5$ with $N=100$ nodes, for the same values of $\alpha$. In both cases we observe a logarithmic growth regime for most values of $\alpha$. The dashed black lines illustrate the regions for $S(t, \alpha)$ remain close to the CTRW value $d_s = 1$ [28]. Thus, for CTRW on a line we obtain $\lim_{\alpha \to 1} d_1(\alpha) = d_s/2 = 1/2$. The spectral dimension of the Sierpinski gasket is also known [1, 28]: $d_s = 2 \ln 3/\ln 5 \approx 1.365$. Thus, for CTRW on a Sierpinski gasket we expect $\lim_{\alpha \to 1} d_1(\alpha) \approx 0.683$, which is larger than the value for the line.

When $\alpha \to 0^+$, the QSW approaches the CTQW. Recent results for discrete-time quantum walks on periodic one-dimensional lattices suggest that the logarithmic growth of the von Neumann entropy in this limit scales with an exponent which is twice as large as the classical random walk exponent [26]. For our analysis this translates to $\lim_{\alpha \to 0^+} d_1(\alpha) \approx d_s = 1$.

Fig. 2 shows $d_1(\alpha)$ for the two structures as a function of $\alpha$. We have extracted the value of $d_1(\alpha)$ from the curves in Fig. 1 by a linear fit in the scaling regions. For both structures we find that $d_1(\alpha)$ increases with decreasing $\alpha$ from 1 to 0.1. For the line the values of $d_1(\alpha)$ remain close to the CTRW value $1/2$ and only start to increase slowly for $\alpha \leq 0.4$, e.g., for $\alpha = 0.1$ we find $d_1(\alpha = 0.1) \approx 0.6$. For smaller values of $\alpha$ there is a steep increase in $d_1(\alpha = 0.1)$ up to values $d_1(\alpha = 0.05) \approx 1$, which is twice as large as the CTRW value. The Sierpinski gasket on the other hand shows a more continuous increase of $d_1(\alpha)$ with decreasing $\alpha$, e.g., for $\alpha = 0.1$ we find $d_1(\alpha = 0.1) \approx 1.4$, which also is about twice as large as the CTRW value. The fact that for both the line and the Sierpinski gasket, the information dimension is ap-
approximately twice as large in the CTQW regime as in CTRW regime, might indicate that this is a more universal feature which certainly needs further investigation, see also Ref. [29] for the discrete-time quantum walk.

In order to corroborate our findings from our phenomenological model, we also compute the von Neumann entropy $S_{vn}(t)$ for a linear chain by using the HEOM. To solve the HEOM we use the program PHI [30, 31]. Due to limited computational resources we take a chain of $N = 9$ nodes and truncate the hierarchy at a depth $M = 14$, corresponding to 497420 auxiliary density matrices. In particular, we have $H_0 = \gamma A^{\text{line}}$, and choose $\gamma = 50 \text{ cm}^{-1}$ and $\Omega = 35 \text{ ps}^{-1}$. The temperature is chosen to be 300K in order to avoid adding low-temperature Matsubara correction terms to the hierarchy [31, 32, 33]. To obtain classical hopping dynamics for large couplings but that it still captures the essential details of the underlying network structure.

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\[ I(\Lambda) = \frac{\Lambda}{500}, \quad \text{where } \Lambda = 500 \text{ cm}^{-1} \]

FIG. 3. Log-linear plot showing the von Neumann entropy $S_{vn}(t)$ obtained with the HEOM for different values of the reorganization energy $\Lambda$ (in units of cm$^{-1}$). The inset shows the area for $\Lambda = 20$, where we fitted the logarithmic growth regime.

In Fig. 2 we show that the information dimension $d_I(\Lambda)$ (blue) has a similar shape as the curve for the QSW. For a qualitative comparison to our QSW results, we have converted $d_I(\Lambda)$ into $d_I(\alpha)$ by assuming that $\alpha = \Lambda/500$, since at $\Lambda = 500 \text{ cm}^{-1}$ the dynamics is purely classical, with $d_I(500) = 0.5$. As mentioned before, due to the small size of the chain it was difficult to extract $d_I(\Lambda)$ for small $\Lambda$. This is why for small $\alpha$, the curve in Fig. 2 does not reach the same value of the information dimension as for the QSW.

To conclude, we have seen that the information dimension $d_I(\alpha)$, obtained from the QSW model, is a very useful quantity for classifying the quantum dynamics on networks in dissipative environments, in contrast to earlier methods such as the average return probability. Additionally, the curves for $d_I(\alpha)$ can give insight into the robustness of the quantum dynamics against environmental noise. By comparing to numerically exact computations, we have shown that this result is not sensitive to the particular implementation of the dissipative process, but that it still captures the essential details of the underlying network structure.

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Here, the environment is modeled in terms of the Caldeira-Leggett model, as a bath of harmonic oscillators that is linearly coupled to the system [34].