Energy transfer in random networks

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Abstract

Recently, the dynamics of excitations in, e.g., ultra-cold Rydberg gases or in light-harvesting complexes, both of which can be modelled by networks, have been of particular interest. Here, the initial excitation (a Frenkel exciton) is created by absorbing a laser excitation or by capturing solar photons. The exciton is transported over the network until it encounters sites where it can get absorbed (the reaction center in the light-harvesting complexes). This process can be modelled by non-hermitian Hamiltonians having complex eigenvalues [1]. In the following, we study (ensemble-averaged) random networks in which the excitation can vanish only at certain (trap) nodes and investigate the survival probability that the exciton does not get trapped during the (quantum) walk [2] over the network. We further show how this is related to the distribution of the imaginary parts of the eigenvalues of the Hamiltonian [3].

Modelling transport

Continuous-time quantum walks

- We model our quantum dynamical system as a network of localized states $|j\rangle$, for $j = 1, \dots N$.
- We identify an unperturbed Hamiltonian $\mathbf{H}_0$ with the connectivity matrix $\mathbf{A}$ [2]:

$$\mathbf{A}_{kj} = \begin{cases} f_j & \text{if } k = j \\ -1 & \text{if } k \text{ and } j \text{ connected} \\ 0 & \text{otherwise.} \end{cases}$$

Here f_j is the number of bonds emanating from j.

Placing a trap into a system

- We take M out of N total nodes to be trap nodes and denote them as m, so that $m \in M$.
- We consider the trapping process with a strength Γ_m by taking a trapping matrix $\mathbf{\Gamma}$: $\mathbf{\Gamma} = \sum_m \Gamma_m (|j\rangle\langle j|)$.
- The total Hamiltonian $\mathbf{H}$ is $\mathbf{H} = \mathbf{H}_0 - i\mathbf{\Gamma}$.
- $\mathbf{H}$ is non-Hermitian and has complex eigenvalues $E_l = \epsilon_l - i\gamma_l$. For small Γ_m, the eigenvalues of the perturbed system are given by:

$$E_l = E_l^{(0)} - i\Gamma_m |\langle m|\psi_l^{(0)}\rangle|^2.$$

Survival probabilities

- The transition probability to go from the node j at time $t = 0$ to the node k at time t is [4]:

$$\pi_{k,j}(t) = \left| \sum_l e^{-i\epsilon_l t} e^{-\gamma_l t} \langle k|\psi_n\rangle \langle \widetilde{\psi}_n|j\rangle \right|^2,$$

where $|\psi_n\rangle$ and $\langle\widetilde{\psi}_n|$ are left and right eigenstates, respectively. The imagionary parts γ_l of E_l determine the temporal decay.

- The mean survival probability $\Pi(t)$ to be at node $k \notin M$ for a total number of M trap nodes is a global property of the network and can be defined as:

$$\Pi(t) = \frac{1}{N - M} \sum_j \sum_k \pi_{k,j}(t).$$

- For long times and a small number of trap nodes, $\Pi(t)$ is a sum of imaginary parts of the eigenvalues E_l:

$$\Pi(t) = \frac{1}{N} \sum_{l=1}^{N} e^{-2\gamma_l t}.$$

- The lower bound of the ensemble-averaged survival probabilities $\langle \Pi(t) \rangle_R$ can be defined with the Jensen's inequality [4]:

$$\langle e^{-2\gamma_l t} \rangle_R \geqslant e^{-2\langle\gamma_l\rangle_R t}.$$

References

[1] O. Mülken, A. Blumen, Phys. Rep. 502 **37** (2011)

[2] E. Farhi and S. Guttman, Phys.Rev. A **58** (1998)

[3] A. Anishchenko et. al., *in preparation*

[4] O. Mülken, A. Blumen, Physica E **42** (2010)

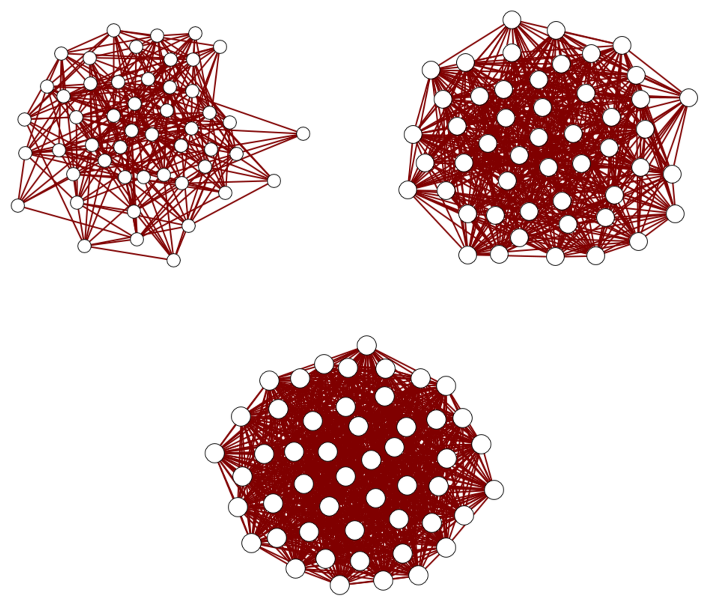
Main results

- For an excitation travelling in a random network, there is still a high probability not to be trapped even at very long times.
- The ensemble-averaged survival probability for an excitation is very near to its lower bound defined with the Jensen's inequality.

Random networks with traps

- We consider random networks $G(N, p)$ which consist of $N = 50$ nodes with probabilities $p = 0.25, 0.5, 0.75$ to be connected.
- For each of $G(50, 0.25)$, $G(50, 0.5)$, and $G(50, 0.75)$, we put a trap into one node, i.e. $m = 1$. We set $\Gamma = 1$.
- We perform $R = 1000$ random realizations of the networks to obtain ensemble-averaged results:

$$\langle \dots \rangle_R \equiv \frac{1}{R} \sum_{r=1}^{R} [\dots]_r.$$



Examples of $G(50, 0.25)$, $G(50, 0.5)$, and $G(50, 0.75)$

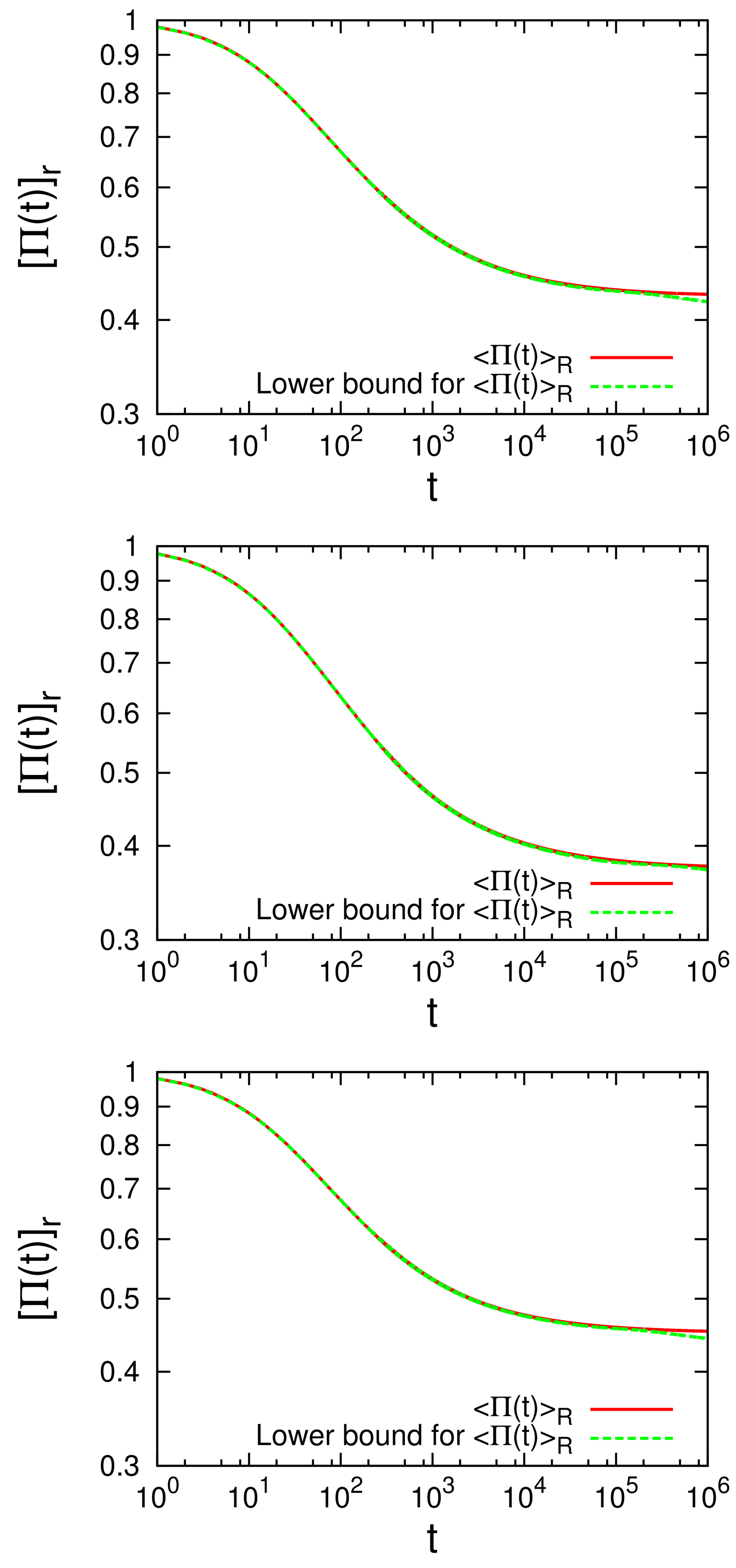
Mean survival probabilities and their lower bounds

- $\langle \Pi(t) \rangle_R$ decays very slowly and converges to a constant value determined by γ_l as:

$$\lim_{t\to\infty} \Pi(t) = \frac{d(\gamma_l = 0)}{N},$$

where $d(\gamma_l = 0)$ is a total number of $\gamma = 0$ in the eigenvaule set of the corresponding $\mathbf{H}$.

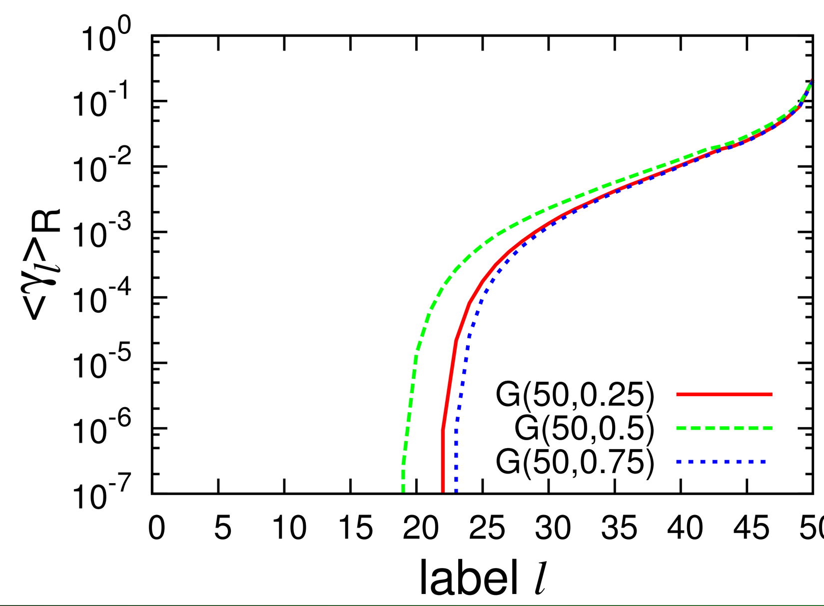
- $\langle \Pi(t) \rangle_R$ does almost coinside with its lower bound.
- Realizations may strongly differ in their behavior displaying stronger and weaker decays.
- There is *a strong localization* at certain eigenstates of $\mathbf{H}$, therefore, $\langle \Pi(t) \rangle_R$ does not vanish even at very long times.



$\langle \Pi(t) \rangle_R$ and their lower bounds for $G(50, 0.25)$, $G(50, 0.5)$, and $G(50, 0.75)$, log-log scale

Eigenvalue sets. Ensemble averages $\langle \gamma_l \rangle_R$ of γ_l

- For some relizations we find $\gamma > 4$ while at most $\gamma << 10^3$ show up. Note the log-lin scale.
- $\langle \Pi(t) \rangle_R$ converges to 18/50 for $G(50, 0.5)$, to 21/50 for $G(50, 0.25)$ and to 24/50 for $G(50, 0.75)$, since $d(\gamma_l = 0) = 18$, 21, and 24, respectively.



Acknowledgments

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