NOISE-INDUCED DETRAPPING IN SMALL QUANTUM NETWORKS*

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Optimizing excitation transport in quantum networks is an important precursor to the development of highly-efficient light-harvesting devices. We investigate the phenomenon of dephasing-assisted leakage from trapped states, which may ensure efficient transport of excitations across a network. We consider three small networks with known trapped states and study the effect of Markovian quantum noise and classical noise sources with different correlation times, from very low frequency non-Markovian noise to white noise. We show that the excitation - otherwise stalled in trapped states - is able to diffuse rapidly through the networks from a source to a sink, with efficiency being generally maximized for intermediate correlation times.

1. INTRODUCTION

Understanding the dynamics of quantum networks is central to the development of quantum computing and communication technologies [1–3]. Quantum control [4] in the presence of noise is an important precursor to improve the efficiency in transferring excitations [5, 6] across quantum networks and has attracted a great deal of interest with regards to information transfer [7], quantum memories [8, 9], quantum phase transitions [10], and the preservation of quantum correlations [11, 12]. In particular in the last few years certain biological light-harvesting structures have been extensively studied since the experimental discovery that an excitation created by an absorbed photon displays wavelike behavior and even long-lasting coherence [13–16]. It has been proposed that both the excitation transfer to a reaction center [5, 6, 17], where it is converted into chemical energy, and the conversion process itself [18] may take advantage of coherence. The problem of transferring an excitation is defined as the time-evolution of an excitation created on a node of a quantum network towards a node acting as a "sink", which represents the reaction Center. It is well known that such networks may support eigenstates localized on only a few nodes, corresponding physically to excitations "coherently trapped" [19], and inhibiting transport. It has been proposed theoretically [5, 6, 20] that dephasing can improve the transport efficiency - a phenomenon called dephasing assisted transport (DAT) - in particular by a detrapping mechanism from the above localized states [5, 21].

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Coherent population trapping is widely studied in driven three-level systems both in quantum optics [19, 22] and in the solid-state [23, 24]. It also occurs in in ordered fully connected networks (FCN) [25] and in disordered small networks. In all these systems investigation of strong or non-Markovian dephasing [21, 26] is the subject of current research. In this paper we study detrapping and transport efficiency in the presence of non-Markovian noise produced by incoherent sources. Since it has been proposed that in general the coexistence of coherence and decoherence due to coupling to an environment may be a key ingredient in optimizing the energy excitation transport in quantum networks [27], we aim to understand the impact of non-Markovianity on quantum transport in solid-state artificial architectures.

In order to elucidate the effects of non-Markovianity we consider relatively weakly coupled noise sources and study the behavior as a function of correlation time, on a range of small networks - the Λ network, a 3-site FCN (Δ network), and a 6-site FCN (FCN6). In particular we study the effect of a bath with an Ornstein-Uhlenbeck (OU) type of temporal correlation, from quasistatic to high frequency noise, finding a non-homogeneous behavior in transfer efficiency. This work complements different studies of effects of non-Markovian noise, such as that produced by an environment of many oscillators beyond the Born approximation [28] or as an unconventional environment containing isolated coherent oscillatory modes [21, 29], which have been investigated with the aim of explaining observations of long-lasting coherence in certain biological complexes.

2. MODEL

We consider a single excitation propagating in a network of N sites. The dynamics is described by the following Hamiltonian,

$$\mathcal{H} = \sum_{i \neq j}^{N} \hbar \Delta_{ij} \left| i \right\rangle \left\langle j \right| + \sum_{i}^{N} \hbar \varepsilon_i \left| i \right\rangle \left\langle i \right|, \tag{1}$$

where $|i\rangle$ represents the excitation (*e.g.* an electron-hole pair) localized on the i-th site, ε_i being the local site energies. Intersite coupling, due for instance to electric dipole interaction, leads to tunneling of excitations where Δ_{ij} is the tunneling amplitude between sites j and i.

We first consider Markovian noise, and model the density matrix dynamics by the Lindblad Master equation [30]:

$$\dot{\rho}(t) = -\frac{i}{\hbar} \left[\mathcal{H}, \rho(t) \right] + \mathcal{L}_{\text{diss}} \left(\rho(t) \right) + \mathcal{L}_{\text{deph}} \left(\rho(t) \right), \tag{2}$$

where the dissipative and dephasing components are given by [21, 31],

$$\mathcal{L}_{\text{diss}}(\rho(t)) = -\sum_{i=1}^{N+1}\sum_{j\neq i}^{N}\frac{\Gamma_{i,j}}{2}\{|j\rangle\langle j|,\rho(t)\}+\sum_{i=1}^{N+1}\sum_{j\neq i}^{N}\Gamma_{i,j}|i\rangle\langle j|\rho(t)|j\rangle\langle i|$$

$$\mathcal{L}_{\text{deph}}(\rho(t)) = -\sum_{i=1}^{N}\frac{\gamma_i}{2}\{|i\rangle\langle i|,\rho(t)\}+\sum_{i=1}^{N}\gamma_i|i\rangle\langle i|\rho(t)|i\rangle\langle i|. \quad (3)$$

The dissipative $\mathcal{L}_{\text{diss}}$ accounts for transitions with rate Γ_{ij} from site j to either a site i or to a sink where the excitation exits the network. The sink is modeled by an irreversible decay into an external site, $i = N+1$, the population of this state being a measure of the energy transfer efficiency. The component $\mathcal{L}_{\text{deph}}$ describes local Markovian dephasing processes. For $\Delta_{ij} = 0$ they determine pure dephasing of localized exciton states, whereas for non-vanishing Δ_{ij} they model transitions between the "dressed" eigenstates $|\phi_n\rangle$ of the Hamiltonian (1), triggered by a high temperature reservoir.

Markovian noise is tackled using the wavefunction approach [30, 32, 33], where the network dynamics are obtained as the average of many quantum trajectories. Each one evolves in general acting with a suitable non-Hermitian effective Hamiltonian, plus transitions from one state to another, accounted for by incoherent quantum jumps generated by a Monte-Carlo algorithm [30].

The dephasing term Eq.(3) describes physically the effect of white noise [31]. However as a rule solid-state systems typically exhibit low-frequency noise, yielding non-Markovian pure dephasing [34]. The simplest instance is "quasistatic noise", which may be physically due to the presence of impurities coupled locally to the network, and is modeled by adding a random variable $\delta\varepsilon_i$ to the ε_i term in the Hamiltonian (1). In general we may add a stochastic process $\delta\varepsilon_i(t)$, and consider

$$\tilde{\mathcal{H}}(t) = \sum_{i\neq j}^{N}\hbar\Delta_{ij}|i\rangle\langle j| + \sum_{i}^{N}\hbar\left[\varepsilon_i+\delta\varepsilon_i(t)\right]|i\rangle\langle i|. \quad (4)$$

In particular we will study the effect of an OU classical stochastic process [35, 36], as discussed later in detail. In order to encompass non-Markovian noise we generalized the numerical wave function approach, considering also different realizations of the stochastic processes. Owing to the fact that the trajectories are independently simulated, averaging over the stochastic process can be performed at the same time, requiring a tolerable computational overhead.

Classical noise is characterized by the un-normalized autocorrelation function, defined as $\mathcal{R}(t') = \langle\delta\varepsilon_i(t)\delta\varepsilon_i(t+t')\rangle$. For the OU process correlations read $\mathcal{R}_{ou}(t') = \sigma_{ou}^2 e^{-t'/\tau}$, where τ is the correlation time. This allows us to interpolate between the two limiting cases and to study effects of Markovian and non-Markovian

Table 1

Summary of the equivalences between the OU process and static noise ($\tau \to \infty$) and white noise ($\tau \to 0$).

Markovian	$\sigma_{ou}^2 = \frac{\gamma}{2\tau}$	$\tau \to 0$
Quasistatic noise	$\sigma_{ou}^2 = \sigma^2$	$\tau \to \infty$

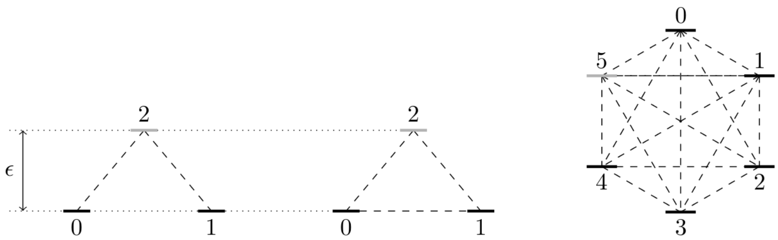

Fig. 1 – Schematic of the Λ (left) and Δ (center) systems and the FCN6 (right). The network is incoherently coupled to the sink *via* the *grey* site.

noise by considering different τ. For Markovian (white) noise there is no correlation over time (correlation time $\tau \to 0$) and $\mathcal{R}_w(t') = \gamma\delta(t')$. In the opposite limit of quasistatic noise ($\tau \to \infty$), $\mathcal{R}_s(t') = \sigma^2$.To find the equivalence between the white noise and the OU process, we compare the area under the autocorrelation functions in the limit $\tau \to 0$. The comparison between the OU process and quasistatic noise occurs in the limit $\tau \to \infty$. The equivalences between parameters in these limits are shown in table 1.

We study three networks, namely the Λ network, the Δ network, and the FCN6 (Fig. 1). In all cases, the dashed lines represent a hopping parameter of $\Delta_{ij} = \Delta_0$ and the system is incoherently coupled to the sink at site N (grey) by the jump rate $\Gamma_{SN} = \Delta_0/10$. In the Λ and Δ networks, site N differs in energy from the other degenerate sites by the on-site energy ϵ, whereas we take equal on-site energies for the sites of the FCN6.

The symmetric Λ and Δ systems and the ordered FCN6 have "trapped" eigenstates of the form,

$$|\phi_i\rangle = \frac{1}{\sqrt{2}}|i\rangle - \frac{1}{\sqrt{2}}|0\rangle, \tag{5}$$

where $i = 1$ in the case of the Λ and Δ systems and$\{i \in \mathbb{Z} | 1 \leq i \leq 4\}$ for the FCN6, *i.e.* such states have no component on site N of the network. They are said to belong to an invariant subspace that will not decay into the sink, thereby the component of the wave function onto these subspaces is "coherently trapped" and cannot escape the network. In the presence of pure dephasing transitions from trapped eigenstates to other delocalized eigenstates enhance the transport efficiency, this being one of the mechanisms of DAT [21].

3. RESULTS

Using the equivalences in table 1, we first check the limits of the OU process by comparing with white noise and static noise sources. Results for the Λ network are shown in Fig. 2. We set $\epsilon = \Delta_0$ and the width of the OU noise source, $\sigma_{ou}^2 = \Delta_0^2$. When the correlation time is large ($\tau = 10^5$), the process approaches the static noise limit, with $\sigma^2 = \sigma_{ou}^2 = \Delta_0^2$. When the correlation time is small ($\tau = 10^{-3}$), the process approaches the white noise limit, where $\gamma = 2\tau\Delta_0^2$. We tune the parameters of the static and white noise sources to values equivalent to the OU process, as indicated in table 1. In both cases, the excitation is initiated in the trapped state, Eq. 5, thereby completely suppressing transport to the sink in the absence of noise.

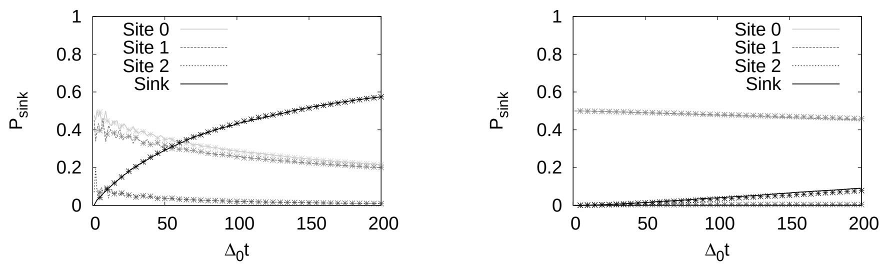

Fig. 2 – Left: Population distribution against time, t, for the Λ network in the presence of static noise (points) and of the equivalent slow OU process (lines); here $\sigma_{ou}^2 = \sigma^2 = \Delta_0^2$ and $\tau = 10^5$. Right: Population distribution within the Λ network in the presence of white noise (points) and of the equivalent fast OU process (lines); here $\sigma_{ou}^2 = \Delta_0^2$, $\gamma = 2\tau\Delta_0^2$ and $\tau = 10^{-3}$. The system is connected to the sink *via* a jump operator acting on site 2, with a rate of $\Gamma_{S2} = 0.1\Delta_0$. In all cases, 10^4 quantum trajectories were used in the simulation.

The left-hand graph of figure 2 shows the equivalence of the OU process for $\tau \to \infty$ with static noise. The equivalence in the Markovian limit is shown by the right-hand graph. In this case the width of the OU process is proportional to the width of the white noise source, but also inversely proportional to the infinitesimal time correlation τ. This means that, if the value γ is of the same order as the value used for σ^2, the noise width of the comparable OU process is prohibitively large. Therefore, for the purposes of this comparison, γ is of the same order of magnitude as τ.

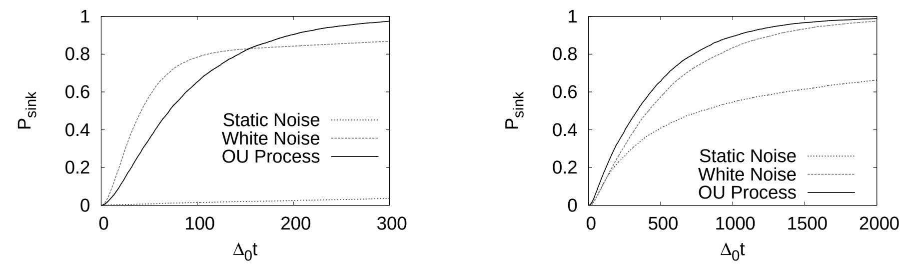

Fig. 3 – Left: Sink population against relative time for the Λ network, for $\sigma^2 = \sigma_{ou}^2 = 0.1\Delta_0^2$, $\gamma = 0.1\Delta_0$, $\epsilon = \Delta_0$, $\tau = \Delta_0^{-1}$. Right: sink population against relative time for the FCN6, with $\sigma^2 = \sigma_{ou}^2 = 0.05\Delta_0^2$, $\gamma = 0.05\Delta_0$, $\tau = \Delta_0^{-1}$. In both cases 10^4 quantum trajectories were used.

We now compare the effects in the above limiting cases with those of a generic OU process with intermediate correlation times. In Fig. 3 (left) we show the population of the sink for the Λ network subject respectively to white noise, quasistatic noise, and generic OU noise. In order to focus on the detrapping phenomenon, we initiate the excitation in the invariant subspace, where it would be trapped in the absence of noise, *i.e.* from a dark state (Eq. 5).

For the Λ network we use $\epsilon = \Delta_0$, and noise is coupled to the operator site $|1\rangle\langle 1|$. We used figures corresponding to relatively weak noise, namely the widths of the OU noise and the static noise are $\sigma_{ou}^2 = \sigma^2 = 0.1\Delta_0^2$, whereas for the white noise we took $\gamma = 0.1\Delta_0$. The quasistatic noise has the smallest effect on the sink population. This is expected, since for low-amplitude noise sources, the initial state has only a small overlap with the sink. Another possible effect of the dephasing is line broadening of the individual site energies. Fluctuations in the site energies over time lead to fluctuations in their energy differences, which directly affects the effectiveness of the transfer rate within the network. Hence, the white noise has a larger effect than static noise on the transport efficiency. It is seen that the OU noise with intermediate correlations has larger effects than the white noise. The main effect in these cases are transitions between eigenstates of the Hamiltonian (1) allowing extended eigenstates to take part to transport.

Results for the FCN6, where all site energies are degenerate, are reported in Fig. 3 (right). For this network weaker figures of noise are taken for the OU, white and static noise, namely $\sigma_{ou}^2 = 0.05\Delta_0^2$, $\gamma = 0.05\Delta_0$, and $\sigma^2 = 0.05\Delta_0^2$ respectively. The excitation is initiated in a superposition of the 4 trapped states (Eq. 5) and the noise sources act to sites 1 to 4, with no correlation between noise acting on different sites. As the system equilibrates, we see again the generic OU process yields a better detrapping, the effect however being only marginally greater than that of white noise.

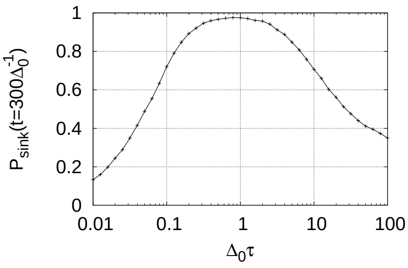

Fig. 4 – Final sink population against correlation time for the Λ network in the presence of the OU process acting on site 1, where $\sigma_{ou}^2 = 0.5\Delta_0^2$ and $\delta = \Delta_0$. The system is connected to the sink *via* a jump operator acting on site 2, with a rate of $\Gamma_{S2} = 0.1\Delta_0$. 10^4 quantum trajectories were used in the simulation.

Static noise is clearly less effective, but population of the sink is more than one order of magnitude larger than for the Lambda network, indicating that static noise may become important for larger systems [37].

In order to address effects of non-Markovianity, we now make a more systematic analysis of the efficiency, given by P_{sink} at a sufficiently large time $t = 300\Delta_0$, as a function of τ (Fig. 4). Here the width of the process is fixed to the value $\sigma_{ou}^2 = 0.5\Delta_0^2$, thereby in all cases the power spectrum for the OU process, given by

$$\mathcal{S}(\omega) = 2\sigma_{ou}^2 \frac{\tau}{1+\omega^2\tau^2}, \tag{6}$$

yields a constant value when integrated over frequencies. The excitation is initiated in the trapped state, Eq. 5. It is seen that the process is most effective when $\tau \approx \Delta_0^{-1}$. Notice that in this regime the noise source neither can be treated by a Markovian master equation nor is quasistatic.

An alternative characterization for different correlation time regimes is to compare noise which would give the same decay time of coherence if treated in by the standard Bloch-Redfield master equation theory [38]. This approach yields microscopic decay rates which are correct in the Markovian limit. A scale for the decay time is $\gamma \sim \mathcal{S}(\Delta_0)$, obtained by arguing that local dephasing triggers transitions between "dressed" eigenstates $|\phi_n\rangle$, whose splitting is $\tilde{\Delta}_0$. To this end, for a given γ we consider a OU process with width σ_{ou}^2 given by

$$\mathcal{S}(\Delta_0) = \gamma \quad \Longrightarrow \quad \sigma_{ou}^2 = \frac{1+\Delta_0^2\tau^2}{2\tau}\gamma. \tag{7}$$

Results are shown in Fig. 5 for the Λ and the Δ network. The final sink population is reported together with the amplitude of coherences at a shorter time, which is slightly larger than $1/\gamma$. Concerning coherences, Eq.(7) implies that if non-Markovianity was unimportant, coherences would not depend on τ, and therefore equal to the value for $\tau \to 0$. Instead we observe an increase of coherences for $\Delta_0\tau > 1$, with only a small effect on the transfer efficiency of the network. This phenomenon is analogous to the "sustained coherence" proposed in Ref. [29] to explain long-lasting coherence in biological complexes. However the OU process studied here shows a much smaller effect, suggesting that sustained coherence stems from strong coupling (in the sense of quantum optics) to an individual environmental mode, semiclassical or quantum, performing sufficiently large oscillation, rather than to non-Markovianity by itself.

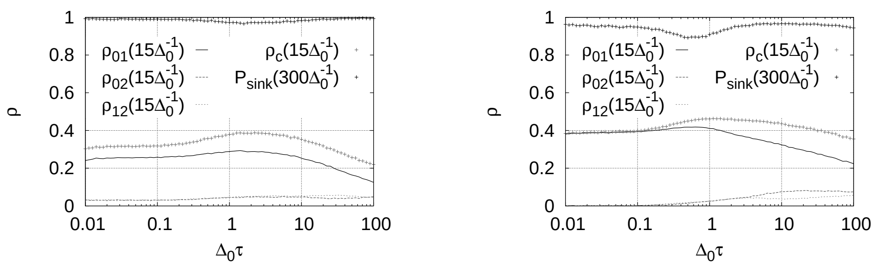

Fig. 5 – Population at time $\Delta_0 t = 300$ and coherences at time $\Delta_0 t = 15$ for the Λ (Left) and Δ (Right) systems. In each case, $\gamma = 0.05\Delta_0$ and $\rho_c = \rho_{01} + \rho_{02} + \rho_{12}$.

4. CONCLUSIONS

We have studied the effect of noise with different correlation times, ranging from very large ones to white noise, on transport of excitations in a collection of small networks - the Λ and Δ networks and the FCN6. The noise is weakly coupled to the system but still sufficient to produce detrapping from the invariant subspace of the Hilbert space of the closed system. As a consequence efficiency of transport towards a sink increases, this being one of the mechanisms of DAT. While in small networks white noise is much more effective than static noise in triggering detrapping, noise determining a non-Markovian dynamical map of the system may be even more effective. We studied systematically the effect of a OU process yielding large DAT for correlation times of the same order of magnitude of the coupling between nodes of the network, $\tau \approx \Delta_0^{-1}$. In slightly larger networks we observed that the relative impact of static noise increases, incentivizing further investigation into larger systems. These results provide insight to design solid-state artificial architectures with improved quantum transport properties.

Models of non-Markovian environments have also been invoked to explain long-lasting coherence in certain biological quantum networks [28, 29]. In order to understand to which extent this phenomenon is related to non-Markovianity we have investigated the effect of a classical stochastic environment. To this end we considered environments with different correlation times, but yielding the same Bloch-Redfield decoherence rate. Although we find that non-Markovianity can sustain coherence for longer times, the effect is small, suggesting that non-Markovianity is not sufficient by itself to explain the phenomenon of long-lasting coherence.

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