Driving the Dephasing Assisted Quantum Transport

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Abstract. Nontrivial quantum effects in biological systems are of high interest among physicists over the past decade. They allow for information and energy to be exchanged with near-unity efficiency despite hindered by the warm, wet, and noisy environment. Several models suggest that the efficient quantum energy transport is due to the interplay between dephasing dynamics and unitary evolution of the disordered biological systems i.e in photosynthetic complex. However, the proposed models have not yet included the driving force depicting the external perturbation used in the experiment such as laser in 2D spectroscopy involved in the detection of the exciton transfer or an artificial quantum transport experiments. Here, we resolve this issue by subjecting the dephasing assisted transport model by Plenio and Huelga\textsuperscript{[New J. Phys. 10, 11 (2012)]} to a driving force. We analyze dynamical evolution of the driven system and show that further efficiency enhancement achieved by driving the transport site. We also discuss some experimental realizations of the quantum transport system.

1. Introduction

Dissipation is usually thought as a detrimental effect in quantum system. However, recent discoveries show that moderate amount of dephasing noise improves the quantum efficiency of exciton transport in biological systems (e.g. photosynthesis) \cite{1}. The so-called environment-assisted quantum transport (ENAQT) \cite{2–5} relies on interplay between coherent (from intersite coupling) evolution and decoherence. Right amount of decoherence can successfully direct the excitation to the trap site (accumulator). The transport mechanism portray a kind of quantum walk in dissipative bath and increased by moderate amount of dephasing \cite{4}. It was thought that ENAQT only exists in disordered system, but in \cite{3} it is proven that ENAQT exist also in any ordered system and the only impossible case is an end-to-end transport (initial site and the trap site is in both ends of a chain-like structure).

The discovery of the ENAQT in photosynthetic systems \cite{1, 6} was striking because even in the warm, wet, and noisy environment the biological system managed to obtain an increase in the energy transfer with an appropriate amount of dephasing and intricate super-molecular structure; a result of million years of natural selection.

Dephasing (environmental fluctuation) is usually hard to control experimentally. We consider an external driving as an appropriate alternative (an extension) to the model. In this paper, we show that periodic driving increases the transport efficiency further. Here we theoretically
model the effect of external driving field applied to the quantum transport aggregate. We are able to give analytical result via rotating-wave approximation in one of two cases considered and compare it to the exact numerical result.

2. The basic setting: ENAQT with on-site driving

We first consider a network of N sites, coupled to each others and may support excitations, which is subject to on-site driving force. The Hamiltonian that describes the setting in one-exciton manifold is given by

\[ H = \sum_{k=1}^{N} (\omega_k + f_k(t))|k\rangle\langle k| + \sum_{k<l} \nu_{k,l} (|k\rangle\langle l| + |l\rangle\langle k|), \]

where we have set \( \hbar = 1 \) Here \( k \) is the site index, \( \omega_k \) is the local site excitation energy, \( \nu_{k,l} \) is the intersite coupling between sites \( k \) and \( l \), and \( f_k(t) \) is the time-dependent driving force which we will specify later. In the next section we will consider the case where the driving \( f_k(t) \) is applied to the coupling terms (off-diagonals).

Environmental effects in ENAQT are modeled by two distinct type of Markovian noise processes of Lindblad type [7]: dissipative process, which reduces the exciton population, is described by the super-operator

\[ D_{\text{diss}}[\rho] = \sum_{k=1}^{N} \mu_k [-\{ |k\rangle\langle k|, \rho \} + |0\rangle\langle 0| \rho |k\rangle\langle k|], \]

where \( |0\rangle \) is a vacuum state. The population-conserving dephasing process, the phase randomization due to vibrational modes of phonon bath, is

\[ D_{\text{deph}}[\rho] = \sum_{k=1}^{N} \gamma_k [-\{ |k\rangle\langle k|, \rho \} + |k\rangle\langle k| \rho |k\rangle\langle k|]. \]

To calculate the transport efficiency, we extend the Hilbert space \( \mathcal{H} \) to contain the trap and vacuum states,

\[ \mathcal{H} = \mathcal{H}_{\text{sites}} + \mathcal{H}_{\text{trap}} + \mathcal{H}_0, \]

where \( \mathcal{H}_0 \) is the space containing zero excitation (vacuum). This extension is not necessary but very useful to verify numerical results. We connect a trap site \( |\text{trap}\rangle \) to the system. For consistency, we also describe the irreversible transfer of exciton population from a specified site \( n \) to the trap with a Lindblad super-operator,

\[ D_{\text{trap}}[\rho] = \kappa [-\{ |n\rangle\langle n|, \rho \} + |\text{trap}\rangle\langle n| \rho |n\rangle\langle \text{trap}|]. \]

Hence the nonunitary evolution of \( \rho \) is completely described by the following Lindblad equation,

\[ \dot{\rho} = \mathcal{L}\rho = -i[H, \rho] + (D_{\text{diss}} + D_{\text{deph}} + D_{\text{trap}})\rho. \]

The efficiency \( \eta \) is defined as the steady-state population of the trap site, that is

\[ \eta = \lim_{t\to\infty} p_{\text{trap}}(t). \]

Likewise the probability off loss is the steady-state vacuum state \( |0\rangle \) population, \( \eta' = \lim_{t\to\infty} p_0(t) \), and by the completeness of the Hilbert space \( \mathcal{H} \) they satisfy \( \eta + \eta' = 1 \) for all \( t \geq 0 \). In the following, we calculate the efficiency for some simple periodic driving. For on-site (diagonal) driving we will numerically integrate the problem to get \( \eta \) for some varying range of driving frequency and dephasing rate. Meanwhile for the coupling (off-diagonal) driving we are able to give analytical approach via effective Hamiltonian obtained with rotating-wave approximation. The analytical efficiency is also compared in section 3.
2.1. Efficiency enhancement of a site-driven ordered linear chain

To study the effect of the driving force, we begin by considering a simple case where the system is ordered ($\omega_k = \omega$) and the sites are identically coupled only with their immediate neighbors ($\nu_{k,l} = v_0\delta_{k,l+1}$ for $k = 1, \ldots, N - 1$) so that the chain is linear. It can be shown that in ordered system the efficiency is independent of the site energy $\omega$ [3]. Hence we shift the site energies to zero, $\omega = 0$. We also take for simplicity $\mu_k = \mu$ and $\gamma_k = \gamma$ for $k = 1, \ldots, N$.

A periodic driving that applied homogeneously to all sites, $f_k(t) = f(t)$ for all $k$, gives no difference to the efficiency $\eta$; in fact it does not effect the population dynamics on the trap site for all time. This behavior occurs because a homogeneous driving force does not give any dynamic disorder to the energy levels of the sites; the system remains ordered at all time. The efficiency of an ordered chain does not depend to the site energies $\omega$ at all, such as shown by analytical calculations in Refs. [3, 8]. Hence, this case is trivial.

We then consider inhomogeneous periodic driving force, here the driving is only applied at a specific site $d$ with

$$f_k(t) = \begin{cases} f_0 \cos(\Omega t) & k = d, \\ 0 & k \neq d. \end{cases}$$

(8)

We take amplitude $f_0 = 1$ since energy can be re-normalized and in this section we take $N = 3$ and the driven site $d = 1$. The excitation is initialized in site 2 and the trap site is connected to site $n = 3$ (see figure 1). Note that ENAQT still occurs in this setting since it is impossible only for end-to-end transport as shown in Ref. [3].

We solve the problem numerically by finding efficiency from steady-state population for some range of parameters. If we choose $\mu = \kappa = 0.1$ and $\gamma = 0.37$ (the optimum ENAQT for the corresponding $\mu$ and $\kappa$) and varying the driving $\Omega$, we obtain some interesting behaviors as depicted in figure 2. One observes that the efficiency $\eta$ peaks at $\Omega$ near 1 and has a global minimum close to the maximum. And when $\Omega$ is large, $\eta$ convergea to 0.217, which is the same efficiency as the non-driven system. This limiting behavior is expected because when $\Omega \to \infty$ the driving is so fast that it averages to zero, as if no driving exist. The prominent feature is that the driving leads to efficiency enhancement in this case, we define this gain as the driving-enhanced open quantum transport $\zeta$,

$$\zeta \equiv \eta_{\text{max}} - \eta_{\infty}$$

(9)

where $\eta_{\infty}$ is when $\Omega \to \infty$ (equivalent to non-driven case).

The case $\Omega = 0$ is equivalent to a static disorder in site frequency. It gives higher $\eta$ than $\eta_{\infty}$ as expected because in this case the dephasing delocalizes the Anderson localization. Meanwhile, the existence of the global minimum is due to destructive interference in the transport sites.
Figure 2: Numerical result with the driving only in site 1 (N=3). The parameters are $\omega = 0$, $\mu = \kappa = 0.1$, and $\gamma = 0.37$. The excitation initiates at site 2.

This portrays an undesired effect if we want an efficiency gain, but this behavior might be useful and deserve some future researches.

However, $\zeta > 0$ does not exist for all $\mu$ and $\kappa$. The general behavior remains elusive because one needs to analytically solve the time-periodic Lindblad equation, Eq. (6), to find the steady state behavior. The Floquet-Markov method might be useful to use in future research to analyze this system.

3. Driving the coupling term

As a comparison to the system in Eq. (1), in this section we curiously analyze how if the driving is applied to the off-diagonals (the coupling term in Eq. (1) to the same system in the previous section. This case gives another interesting behavior and we can find an approximation to give analytical solution to describe the approximate general behavior.

Consider the following Hamiltonian,

$$H = \sum_{k=1}^{N} \omega_k |k\rangle \langle k| + \sum_{k<l} \nu_{k,l} (|k\rangle \langle l| + |l\rangle \langle k|) f_k(t).$$

In contrast to Eq. (1), here the driving is applied such that the coupling between sites vary in time. In this paper we consider a site-uniform periodic driving,

$$f(t) = \cos(\Omega t).$$

This means that the couplings between adjacent sites are oscillating in strength.

3.1. Analytical solution: rotating-wave approximation

To do rotating-wave approximation one omits the fast-oscillating part in the Hamiltonian. In our case these are terms with $\exp(n\Omega t)$ with $n > 1$. In this case for $N = 3$ we are able to find a rotating frame suitable for applying the approximation. Consider the Hamiltonian in rotating-frame

$$H' = U^\dagger H U + iU^\dagger \frac{dU}{dt}$$

with unitary transformation

$$U = \exp(iS_z \Omega t)$$

where \( S_z = \text{diag}(1, 0, -1) \) is the usual spin representation for spin-1 particles. To understand the approximation, here we explicitly write the rotating-frame Hamiltonian:

\[
H'(t) = \begin{pmatrix}
\omega - \Omega & e^{-i\Omega t} \nu \cos(\Omega t) & 0 \\
e^{i\Omega t} \nu \cos(\Omega t) & \omega & e^{-i\Omega t} \nu \cos(\Omega t) \\
0 & e^{i\Omega t} \nu \cos(\Omega t) & \omega + \Omega
\end{pmatrix}.
\] (14)

Now we can set the terms \( \exp(\pm 2i\Omega t) \) in the off-diagonals so that the Hamiltonian is time-independent. The time independence is important because \( \eta \) is calculated by solving the steady state condition, we use the following method by ref. \[3\] to get nontrivial solution. We solve the following system of linear equations for the steady-state solution \( \rho_{ss} \):

\[
\mathcal{L}\rho_{ss} = \lim_{\epsilon \to 0} \epsilon \rho(0).
\] (15)

Bear in mind that \( \rho \) is a 5x5 matrix for \( N = 3 \) (c.f the total Hilbert space in Eq. (4)). Thus, the efficiency \( \eta \) is trap site part of \( \rho_{ss} \) (the only non-zero component). This lead to a rather tedious Gaussian reduction whose result is not shown here.

However, rotating-wave approximations are credible only for large driving frequencies. It will be shown in next section by comparing the analytical calculation to exact numerical result.

### 3.2. Exact numerical solution

We compare the analytical result above with an exact numerical treatment. With the same parameters as in figure 2, we get the result in figure 3. It is obvious that in figure 3, the rotating-wave approximation missed the intriguing oscillating pattern for small \( \Omega \) and only accurate for large \( \Omega \). However, the analytical peak exists close to the numerical global maximum. The complete explanation for the emergence of still pattern remains elusive, but nevertheless we can analyze the time evolution (figure 3b) for the initial excitation site to gain understanding of what is behind the transport efficiency gain.

Figure 3b shows that for optimum driving enhancement \( \zeta \), in this case by \( \Omega = 0.766 \), the interference pattern has two alternating peaks similar to quantum beatings (as a result of frequencies combined) and its population reduces the fastest. While for large driving, \( \Omega = 5 \) the driving completely dominates the evolution so that it never reaches zero (meaning the population inversion is never happened). In this case the efficiency tends to zero.

The oscillating behavior in figure 3a might result due to the variation of beating patterns such as in figure 3b for \( \Omega = 0.766 \). The driving-enhanced open quantum transport is about 0.05 in this setting. However, further clarification is needed to explain these interesting behaviors.

### 4. Experimental realizations

Over the last decade, simulations of quantum transport is already made feasible in laboratory experiments. For instance, the transport of the chain of Rydberg atoms [9, 10] and chain of trapped ions [11]. While serving a vast array of research topics, those two experiments can act as a simulator of a more complex system such as photosynthetic energy transfer that cannot be directly accessible to quantum optical experiments. Recently, the simulator for quantum energy transport with Rydberg aggregates is proposed [12]. In virtue of the simulator, one have a highly controllable experimental setup to study the evolution of systems whose Hamiltonian are the same (or at least approximately) to the simulator’s.

### 5. Conclusion

We have shown the role of external periodic driving to the environment-assisted quantum transport (ENAQT) for two cases. The first is on-site driving where uniform driving yields
Figure 3: Exact numerical results for $N = 3$ with off-diagonal driving. Same parameters as in figure 2. (a) The efficiency oscillates logarithmically in driving frequency and has a global maximum in $\Omega = 0.776$. The driving-enhanced open quantum transport (OQT) is shown. (b) Time evolution of the driven system. Beating pattern exists for optimum transport and population inversion does not exist in large $\Omega$, see text.

trivial result. Driving only one of the sites instead will give an enhancement in transport efficiency over some range of dissipative, trapping, and dephasing parameters. The second case is off-diagonal (coupling) driving which yields an interesting oscillating pattern; we obtain the analytical result via rotating-wave approximation. We leave some open questions of how exactly the enhancement mechanism work in presence of external driving. This needs further scrutiny of analytical calculations of steady states of a periodic open quantum systems.

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