Models of decoherence-assisted transport in quantum networks

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Abstract. The dynamics of a quantum network under the influence of decoherence were studied. This work is a generalisation of previous research on decoherence-assisted transport in a dimer system [I. Sinayskiy, A. Marais, F. Petruccione and A. Ekert, Phys. Rev. Lett. 108, 020602 (2012)]. The model under investigation consists of a homogenous fully connected quantum network in contact with an environment of spins. Exact analytical expressions for the transition probabilities are obtained. It is shown that there exist well-defined ranges of parameters for which decoherent interaction with the environment assists energy transfer in the quantum network. This model of decoherence-assisted energy transfer is applied to energy transfer in the Fenna-Matthews-Olson complex.

1. Introduction

Recently, evidence of quantum coherence has been detected in biological systems at physiological temperature, including the photosynthetic light-harvesting complexes of a species of green sulphur bacteria [1] and two species of marine cryptophyte algae [2]; organisms well-adapted to photosynthesise under low-light conditions. Light-harvesting complexes act as antennas, absorbing photons and transferring the resulting excitation energy through a network of photoactive pigments held in well-defined orientations and configurations by a scaffold of proteins, to the reaction centre, where the secondary photosynthetic process of charge separation takes place. The electronic excitation energy transfer (EET) happens on a scale of picoseconds and with a quantum efficiency of over 95% [3]. The surprising phenomenon of quantum coherence in warm, noisy, complex and yet remarkably efficient energy transfer systems has led to discussion about the role of the protein environment in the energy transfer process and the degree to which it may contribute to this efficiency [4].

Modelling the complexity of the environment is a challenge. The protein-solvent environment interacts strongly with the pigments due to its polarity and as a result can have a significant effect on the quantum dynamics, which will therefore in general be non-Markovian [5]. Such non-Markovian effects have widely been taken into account [5, 6], but so far, all have been within spin-boson models of excitons within a protein medium. While any biological system is always in contact with a bosonic environment, interaction with a more structured environment such as a spin bath is more likely to assist quantum efficiency and also induces intrinsically non-Markovian dynamics [7].

With the aim of exact solvability, we investigate the relationship between environmental spin degrees of freedom and the efficiency of the EET process described by the Hamiltonian H_{ex}

$$H_{ex} = \sum_j E_j |j\rangle\langle j| + \sum_{i\neq j} V_{ij} |i\rangle\langle j|, \tag{1}$$

where the site energies of the pigments are given by E_j, and the EET couplings by V_{ij}. We review the case of the dimer system; generalise this model to a fully connected network; and finally apply this model to the Fenna-Matthews-Olson (FMO) antenna complex [10].

2. Dimer

For a dimer with Hamiltonian $H_d = \varepsilon_1|1\rangle\langle 1| + \varepsilon_2|2\rangle\langle 2| + J(|1\rangle\langle 2| + |2\rangle\langle 1|)$, the maximum transfer probability for a single excitation $\mathrm{Max}[P_{1\to 2}(t)]$ is given by $J^2/(J^2+\Delta^2)$ where J is the amplitude of transition, and the detuning Δ is given in terms of the energy levels of the dimer as $(\varepsilon_2 - \varepsilon_1)/2$. Certain transfer is achieved when $\Delta = 0$ at time $t = \pi/(2J)$, or when there is resonance between the energy levels in the system.

In a recent article [8], it is shown that there exist well-defined ranges of parameters for which a purely decoherent interaction with environmental spins in a spin star configuration [7] assists energy transfer in the dimer system. For a dimer with each level coupled to a spin bath at zero temperature, the Hamiltonian of the total system is given by

$$H = H_d + H_B + H_I. \tag{2}$$

Each environment B_j consists of n_j spin-half particles

$$H_B = \sum_{j=1}^{2} H_{B_j} = \sum_{j=1}^{2}\sum_{k=1}^{n_j} \alpha_j \frac{\sigma_z^{k,j}}{2}, \tag{3}$$

where $\sigma_z^{k,j}$ are Pauli matrices. The purely decoherent interaction between each site j in the system and the corresponding spin bath is modelled by

$$H_I = \sum_{j=1}^{2} H_{I_j} = \sum_{j=1}^{2}\sum_{k=1}^{n_j} \gamma_j |j\rangle\langle j| \frac{\sigma_z^{k,j}}{2}. \tag{4}$$

The Hamiltonian of the environment H_B commutes with the Hamiltonian of interaction H_I and therefore the state of the total system is always in a product state of the network and the baths. As a result, the effective Hamiltonian for the total system with spin baths at zero temperature is given by

$$H = \sum_{j=1}^{2} \varepsilon'_j |j\rangle\langle j| + \sum_{\substack{i,j=1\\ i\neq j}}^{2} J|i\rangle\langle j|, \tag{5}$$

where $\varepsilon'_j = \varepsilon_j - \gamma_j n_j/2$.

For the Hamiltonian H, the maximum transfer probability $\mathrm{Max}[P_{1\to 2}(t)]$ is given by $J^2/(J^2 + \Delta'^2)$ where in this case the detuning is given by $\Delta' = (\varepsilon'_2 - \varepsilon'_1)/2$, and ε'_j are the shifted energy levels of the dimer as a result of coupling with strength γ_j with each of the spin baths with

number of spins n_j. Certain transfer is similarly achieved when $\Delta' = 0$, which in this case is possible for a wide range of the parameters γ_j and n_j.

This effect persists at physiological temperature, where transfer probabilities of nearly 90% can be achieved in the dimer at 300 K for biologically relevant parameters [8].

3. Fully-connected quantum network

For a fully connected network of N qubits interacting via homogeneous Heisenberg XX coupling with coupling strength $2J$ and with equal site energies ε, the effective Hamiltonian in the single excitation subspace is given by

$$H_N = \sum_{i=1}^{N} \varepsilon |i\rangle\langle i| + \sum_{\substack{i,j=1 \\ i\neq j}}^{N} J|i\rangle\langle j|. \tag{6}$$

By coupling $N-k$ of the sites in the fully connected network to independent spin environments in symmetric star configurations, the Hamiltonian of the total system is given by

$$H_k = H_N + H_B + H_I, \tag{7}$$

with H_B and H_I defined as previously, but with $j = 1, ..., N-k$. We can then write the effective Hamiltonian for the total system, with the baths arbitrarily coupled to the last $N-k$ sites, as

$$H_k = \sum_{j=1}^{k} \varepsilon |j\rangle\langle j| + \sum_{j=k+1}^{N} \varepsilon_j |j\rangle\langle j| + \sum_{\substack{i,j=1 \\ i\neq j}}^{N} J|i\rangle\langle j|, \tag{8}$$

where $\varepsilon_j = \varepsilon - \gamma_j n_j/2$.

In the case where $k = N$ and all levels have equal energy ε, the Hamiltonian H_N is given by Eq. (1). In this case the maximum probability of purely coherent transfer through the network is

$$\mathrm{Max}[P_{I\to F}(t)] = \frac{4}{N^2}, \tag{9}$$

at time $t = \pi/(NJ)$. Our study will focus on whether decoherent interaction between a fully-connected network and environmental spins can enhance energy transport through the network.

We analyse a range of cases where spin baths are added to the initial, final and intermediate network sites, and find that decoherent interaction with the spin baths in general increases transfer probability through the network, and furthermore that these effects persist at physiological temperature [9].

As an example, we consider here the case of coupling both the initial and final sites to spin baths, with Hamiltonian H_{N-2} given by Eq. (8) with $k = N-2$. In this case, it can be shown that when the shifted energy levels are equal, $\varepsilon_1 = \varepsilon_2$, there exist times for which the transfer probability is arbitrarily close to 1.

We now show that such an effect persists at physiological temperatures by considering the Hamiltonian H_{N-2} with spin baths at a temperature of 300 K coupled to the initial and final sites.

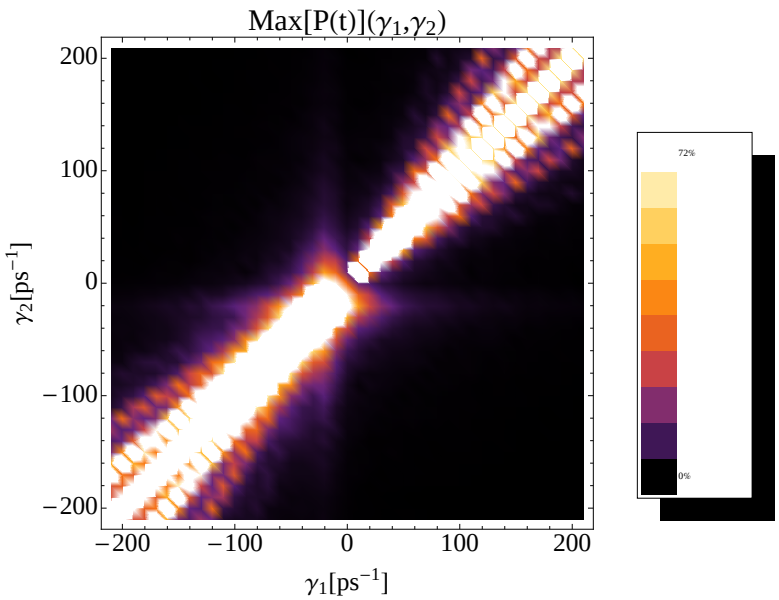

Figure 1. Graph of the maximum of the probability of transition $\mathrm{Max}[P_{I\to F}(t)]$ at 300 K in a 10-site fully connected homogeneous network, with isolated site energies $\varepsilon = 100\mathrm{ps}^{-1}$, and spin baths coupled to each of the initial and final sites, with $n_1 = n_2 = 10$ and bath energy parameter $\alpha_1 = \alpha_2 = 100$ ps^{-1}.

In this case the initial state of the bath is given by the canonical distribution

$$\rho_B(0) = \prod_{i=1}^{2} \frac{1}{Z_i} \mathrm{e}^{-\beta\alpha_i S_i^z}, \tag{10}$$

where Z_i is the partition function of the corresponding spin bath, β is the inverse temperature and S_i^z are collective spin bath operators, see [8] for details.

In Fig. 1 the maximum of the probability of transition $\mathrm{Max}[P_{I\to F}(t)]$ for such a system is plotted as a function of the coupling constants γ_1 and γ_2 with spin baths coupled to each of the initial and final sites. It can be seen that in regions where $\varepsilon_1 \approx \varepsilon_2 \neq \varepsilon$, transfer probabilities of up to 72% are achieved.

4. FMO complex

The first evidence of quantum coherence in photosynthetic antennas at physiological temperature was detected in green sulphur bacteria and cryptophyte algae [1, 2], both organisms able to photosynthesise efficiently at low light intensities. Green sulphur bacteria uniquely contain a complex called the Fenna-Matthews-Olson (FMO) complex [10], which mediates excitation energy transfer from the antenna to the reaction centre [11]. The site energies and optical transition energies for the FMO complex of *Chlorobium tepidum* used here were calculated by Adolphs and Renger [12]. Quantum coherent EET through the bare excitonic system without adding environmental contributions to the Hamiltonian H_{ex}^{FMO} happens with a low probability: for the transfer of the excitation from site 1 to site 3, the probability of transfer is just 4.2%.

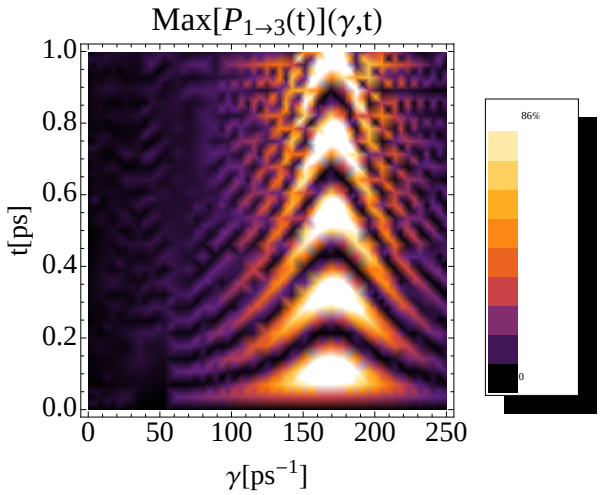

Figure 2. The probability of transfer $P_{1\to3}(\gamma, t)$ for the FMO complex with sites coupled to spin baths at 300 K with numbers of spins at each site $n_1 = 2, n_4 = 8$ and $n_{2,3,5,6,7} = 0$ and spin bath energy constant α=150 ps^{-1}. The maximum transfer probability is 86%.

We now investigate the effect of decoherent interaction with environmental spins at 300 K on the process of EET in the FMO complex.

With the spin baths at a temperature of 300 K, we calculate the maximum probability of transfer during the first picosecond, for equal environmental couplings γ between 0 and 250 ps^{-1} at each site. We find that for a total of 10 spins, distributed between the seven network sites as follows: $n_1 = 2, n_4 = 8$ and $n_{2,3,5,6,7} = 0$, and with spin bath energy constant α=150 ps^{-1}, the maximum transfer probability is 86% (see Fig. 2). This is a vast increase in the transfer probability from the case with no spin baths, where the probability is 4.2%. Therefore, in this case decoherence assists the efficiency of quantum coherent EET in the FMO complex.

5. Conclusion

The recent detection of quantum coherence in biological systems that are remarkably efficient in transferring excitation energy at physiological temperatures, has led to the investigation as to whether this coherence contributes to the efficiency. Here, we have investigated the influence of environmental spins on quantum coherent transfer. We have shown through the derivation of analytical expressions that the transfer probabilities through a fully connected quantum network are improved as a result of decoherent interaction with environmental spins, and that in some cases certain transfer can be achieved. Moreover, this effect is shown to persist at physiological temperatures. We apply this model to the FMO complex, and find that coupling the network sites with environmental spins at physiological temperature improves transport through the network for the considered case. These promising results motivate further study of biological transport systems where environmental spins may play an important role in the dynamics.

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