Coherent versus incoherent energy transport: Effects of harmonic deformations

Naghi Behzadi [a] *, Bahram Ahansaz [a b] †

[a]Research Institute for Fundamental Sciences, University of Tabriz, Tabriz, Iran,

[b]Department of Physics, Shahid Madani University of Azarbayijan, Tabriz, Iran.

January 5, 2016

Abstract

In this work, we study the effects of coherent and incoherent transport of energy through two types of configurations of four interacting two-level systems. Both of the configurations are irreversibly attached to the respective reaction centers. For the first type, the dynamics is only coherent, while for the second one the coherent evolution is completely suppressed and the evolution of the system is only incoherent induced from interaction of the system with fluctuating environments. We calculate the efficiency of transport for both of the configurations in the presence of harmonic deformations. It is found that for a special type of deformations, the efficiency of incoherent transport becomes better than the coherent one.

PACS Nos:
Keywords: Coherent transport, Incoherent transport, Harmonic deformations, Dephasing noises.

1 Introduction

Transport phenomena have been central to quantum mechanics since its early days. Recently it has been renewed by the prospect of transferring quantum information across quantum networks [1, 2, 3, 4] and the recurring interest in understanding the fundamental processes influencing energy transport in photosynthetic systems [5, 6, 7, 8, 9]. The presence of environmental noises is generally considered to be an unavoidable hindrance to efficient transport of charge or energy through quantum systems and the general view is that transport in quantum systems relies on their coherence which is inevitably reduced by interactions with an external noisy environment. However, inspired by the experimental results, further theoretical studies of energy transport in light harvesting complexes have been carried out that

*E-mail:n.behzadi@tabrizu.ac.ir
†E-mail:b.ahansaz@azaruniv.edu

investigate the role of noises, and in particular dephasing ones, in the process of exciton transport in these complexes [10, 11, 12, 13]. Indeed, the efficient transport observed in certain biological systems is not compatible with a fully coherent evolution, so in this way, interplaying between coherent (unitary) dynamics and incoherent (irreversible) dynamics gives the optimal way for quantum transport in many noisy systems. Recently it has begun to be appreciated that vibrational modes arising in molecular structures may play an important role in the dynamics of such systems [14, 15]. Particularly, at room temperature, what is clear is that exciton energy transport depends not only on the topology of electronic couplings among sites but also on the simultaneous effects of the molecular motions and environmental fluctuations which drive efficient transport processes. Also, collective vibrational motions which may arise through a coupled many-body quantum system can lead to an enhancement in the transport of excitations across such systems [16, 17].

On the other hand, the optimal mixing of coherent and incoherent quantum transport is dependent on the initial state preparation [18, 19]. In Ref. [18], it was shown that the optimal transport of excitation through a linear chain when the excitation is initially prepared in one of ends of the chain, is only coherent. In other words, optimal transport is obtained by only self evolution of the system. Also, in Ref. [20], incoherent quantum transport in regular networks has been investigated where the coherent transport, due to the destructive interferences, is completely suppressed. In this case, the optimality of the incoherent quantum transport is dependent on the optimal effects of dephasing noises.

In the present work, we consider two configurations which each of them composed of four two-level atoms with the same geometries and with an additional sink site attached to them respectively. For the first configuration, the optimal dynamics is only coherent, while for the second one is only incoherent, which in turns, related to the optimal effects of dephasing noises on the system. In this situation, we consider some harmonic deformations on the geometry of configurations and highlight their effects on the respective efficiency of transports. It is shown that, in the absence of harmonic deformations, the efficiency of coherent transport is better than the incoherent one which is in accordance with the results of Ref. [18]. However, in the presence of harmonic deformations, it is observed that the efficiency of incoherent transport can be improved to be better than the coherent one. These results, in turn, ensure the point that the induced evolutions can be more effective than the self evolutions of a system, the fact that can be observed in biological systems.

This paper is organized as follows: In section 2, we demonstrate the basic ingredients for achieving the optimal coherent and incoherent quantum transport through two types of configurations with fixed vertices, along with making a comparison between them. Section 3 is devoted for describing the various useful harmonic deformations which can be occurred in the structure of configurations and explaining their effects on the respective efficiency of coherent and incoherent quantum transport. Finally, a brief conclusion is presented in section 4.

2 The model

The general Hamiltonian describing the energy transport of an excitation through a network composed of four two-level quantum system, as depicted in Fig. 1(a) and Fig. 2(a), is given as follows

$$H = \sum_{i=1}^{4} \hbar\omega_i \sigma_i^+ \sigma_i^- + \sum_{\{i,j\}\in E} \hbar J_{i,j} \left(\sigma_i^- \sigma_j^+ + \sigma_i^+ \sigma_j^-\right), \tag{1}$$

where $\sigma_i^+ = |i\rangle\langle 0|$ and $\sigma_i^- = |0\rangle\langle i|$ are the raising and lowering operators for a two-level system lied at ith vertex of the network with transition frequency ω_i. We assume that the atoms are identical and so we have $\omega_1 = \omega_2 = \omega_3 = \omega_4 = \omega$. The strength of coupling between the ith and jth atoms is denoted by $J_{i,j}$ which indicates the hopping rate of excitation between them. E is the set of edges of the network, corresponding to the coupling between the sites as shown in Fig. 1(a) and Fig. 2(a). We consider a configuration in which the all of the coupling constants are equal to each other, i.e. $J_{1,2} = J_{1,3} = J_{2,4} = J_{3,4} = J$ (see Fig. 1(a)). This consideration is corresponding to the configuration in which the optimal dynamics is coherent. To clarify this point, let's introduce a new set of basis as [21] as follows

$$|s_1\rangle := |1\rangle, \quad |s_2\rangle := \tfrac{1}{\sqrt{2}}(|2\rangle + |3\rangle), \quad |s_3\rangle := |4\rangle, \tag{2}$$

where $|s_1\rangle$, $|s_2\rangle$ and $|s_3\rangle$ are basis correspond to the three column of Fig. 1(a) (see Ref. [21]). The Hamiltonian (1) in this basis becomes as

$$H = \sqrt{2}J(|s_1\rangle\langle s_2| + |s_2\rangle\langle s_3|) + h.c.. \tag{3}$$

Clearly, (3) is similar to the Hamiltonian of a chain of three site with equal coupling $\sqrt{2}J$ (see Fig. 1(b)). As denoted in Ref. [18], for this configuration, if the excitation is initially prepared at site 1, the coherent evolution is the optimal dynamics in transferring it to the sink or reaction center.

Now let‘s consider the other configuration in which for the coupling constants we have: $J_{1,2} = J_{1,3} = J_{2,4} = -J_{3,4} = J$ (see Fig. 2(a)). By this assumption, we introduce another set of basis in the single excitation subspace, [2, 3, 4, 20], as

$$|s_1\rangle := |1\rangle, \quad |s_1^{\pm}\rangle := \tfrac{1}{\sqrt{2}}(|2\rangle \pm |3\rangle), \quad |s_2\rangle := |4\rangle. \tag{4}$$

The Hamiltonian (1), indeed, is left with a direct sum structure as

$$H = H_1 \bigoplus H_2, \tag{5}$$

where

$$\begin{aligned} H_1 &= \sqrt{2}J(|s_1\rangle\langle s_1^+| + |s_1^+\rangle\langle s_1|), \\ H_2 &= \sqrt{2}J(|s_1^-\rangle\langle s_2| + |s_2\rangle\langle s_1^-|), \end{aligned} \tag{6}$$

and the respective invariant subspaces are denoted as follow

$$\begin{aligned} \mathcal{H}_1 &= \mathrm{span}\{|s_1\rangle, |s_1^+\rangle\}, \\ \mathcal{H}_2 &= \mathrm{span}\{|s_1^-\rangle, |s_2\rangle\}. \end{aligned} \tag{7}$$

It is well-known that, for this configuration, coherent evolution can not transfer the excitation from site 1 to the reaction center (see Fig. 2(b)). Because the coherent evolution of the system is restricted only in the invariant subspace $\mathcal{H}_1$, and therefore, the existence of induced or incoherent evolution arisen from interaction of the system with fluctuating environments, which conserves the energy, is necessary. We consider, without lose of generality, that the system interacts with the structureless environments through the sites 2 and 3. Therefore, in the Markovian approximation, the effects of these interactions on the dynamics of the system, called dephasing noises, are described by the following Lindblad super-operator

$$\mathcal{L}_{deph}(\rho) = \sum_{i=2}^{3} \gamma_i (2\sigma_i^+ \sigma_i^- \rho \sigma_i^+ \sigma_i^- - \{\sigma_i^+ \sigma_i^-, \rho\}), \tag{8}$$

where γ_js are the rates of dephasing noises which randomize the phases of local excitations and $\{A, B\} := AB + BA$. In order to measure how much of the excitation energy is transferred along the network, we introduce an additional site, the sink, that connected to site 4. The sink is populated by an irreversible decay process from a chosen site as described by

$$\mathcal{L}_{sink}(\rho) = \Gamma(2\sigma_5^+ \sigma_4^- \rho \sigma_4^+ \sigma_5^- - \{\sigma_4^+ \sigma_5^- \sigma_5^+ \sigma_4^-, \rho\}), \tag{9}$$

where Γ is the rate of dissipative irreversible process that reduces the number of excitations in the system. Therefore, the population of the sink referred as efficiency of transport, is given by

$$P_{sink}(t) = 2\Gamma \int_0^t \rho_{4,4}(t') dt'. \tag{10}$$

We note, in this paper, that the Lindblad operators are time-independent and the dephasing rates are positive, i.e. $\gamma_j \geq 0$, therefore the dynamics for the second configuration, as an open system, can be described by time-independent Markovian master equation in the following Lindblad form [22]

$$\frac{d\rho}{dt} = -i[H, \rho] + \mathfrak{L}(\rho), \tag{11}$$

where $\mathfrak{L}(\rho) = \mathcal{L}_{deph}(\rho) + \mathcal{L}_{sink}(\rho)$. Remember that, the term $-i[H, \rho]$ is responsible for the transfer of excitation to the reaction center in the first configuration, while in the second configuration this task is performed by the term $\mathcal{L}_{deph}(\rho)$. When all of the sites are fixed, both of the systems are initially prepared with a single excitation localized at the site 1, i.e. $\rho(0) = |1\rangle\langle 1|$, and it is assumed that, $\gamma_2 = \gamma_3 = \gamma$ and $\Gamma = 2\gamma$. For the second system, the maximal efficiency of incoherent transport is occurred for the optimal value of dephasing rate $\gamma = \gamma_{opt} = 1.05$. Fig. 3, shows the population of the sink versus time for both systems. It is clear that the optimal efficiency of coherent transport is more than the optimal efficiency of incoherent transport. This observations is in complete agreement with results of Refs [18].

3 Effects of harmonic deformations

We consider the harmonic deformations as mechanical oscillations of the vertices around their respective equilibrium positions which change their relative distance and therefore, modulate the distance-dependent dipolar coupling. Time-dependent distance between the sites i and j is as follows

$$d_{i,j}(t) = d_0 - [u_i(t) - u_j(t)] = d_0(1 - 2a_{i,j}sin(\omega_0 t + \phi_{i,j})) \tag{12}$$

where d_0 is the equilibrium distance between two connected sites, u_i is the displacement of the ith site from its equilibrium position and $a_{i,j}$ is the individual relative amplitude of oscillations of sites ith and jth when they move with opposite phase around their equilibrium positions. The dipole-dipole coupling between the sites i and j has the form [17] as

$$J_{i,j}(t) = \frac{\tilde{J}_0}{[d_{i,j}(t)]^3} = \frac{J_0}{(1 - 2a_{i,j}sin(\omega_0 t + \phi_{i,j}))^3}, \tag{13}$$

where $\tilde{J}_0$ contains the dipole moments and physical constants, and we define $J_0 = \tilde{J}_0/d_0^3$, which has the units of energy. Henceforth, all energies, time scales and rates will be expressed in units of J_0. Therefore, by existence some time-dependent coupling strength such as $J_{i,j}(t)$, the equation (1) represents a time-dependent Hamiltonian.

We consider deformations for which the conditions, $J_{1,2}(t) = J_{1,3}(t) \equiv \zeta_1(t)$ and $J_{2,4}(t) = \pm J_{3,4}(t) \equiv \zeta_2(t)$, are satisfied for all of times (+ is devoted for the coherent evolution of the first configuration and - for the incoherent evolution of the second system). Therefore, the deformed time-dependent Hamiltonian for the coherent evolution becomes as

$$H(t) = \sqrt{2}\zeta_1(t)(|s_1\rangle\langle s_2| + |s_2\rangle\langle s_1|) + \sqrt{2}\zeta_2(t)(|s_2\rangle\langle s_3| + |s_3\rangle\langle s_2|), \tag{14}$$

and for the incoherent one becomes as $H(t) = H_1(t) \bigoplus H_2(t)$, with

$$\begin{aligned} H_1(t) &= \sqrt{2}\zeta_1(t)(|s_1\rangle\langle s_1^+| + |s_1^+\rangle\langle s_1|), \\ H_2(t) &= \sqrt{2}\zeta_2(t)(|s_1^-\rangle\langle s_2| + |s_2\rangle\langle s_1^-|). \end{aligned} \tag{15}$$

By these considerations, the time-independent Markovian master equation (11) becomes a time-dependent one for the description of the incoherent evolution of the second configuration. When only the site 1 oscillates around its equilibrium along the horizontal line connecting the sites 1 and 4, then $\zeta_1(t) = J_{1,2}(t) = J_{1,3}(t)$ varies oscillatory with time, while, $\zeta_2(t) = J_{2,4}(t) = \pm J_{3,4}(t) = 1$, is constant (see Fig. 4(b)). For this case, the optimal efficiency of transport for the coherent and incoherent transfer of excitation from site 1 to the sink, with respect to time, is shown in Fig. 4 (a). In contrast to the case shown in Fig. 3, we see particularly that, as time goes on, the optimal efficiency of incoherent transport becomes better than the coherent one. Now let's only the site 4 oscillates, similar to the oscillation of site 1 in the previous case, such that $\zeta_1(t) = J_{1,2}(t) = J_{1,3}(t) = 1$ and $\zeta_2(t) = J_{2,4}(t) = \pm J_{3,4}(t)$ (Fig. 5(b)). Fig. 5(a), shows that the optimal efficiency of transport for the coherent and incoherent evolutions are completely different from those that depicted in Fig. 4(a). It is, indeed, hard to judge that the efficiency of incoherent transport is more favorable than the coherent one.

The interesting instance that witnesses the superiority of incoherent transport on the coherent one is occurred when the sites 1 and 4 oscillate simultaneously with phase difference

$\Delta\varphi = \pi$ along the horizontal line so both of $\zeta_1(t)$ and $\zeta_2(t)$ change differently with time as shown in Fig. 6(b). As time grows, in optimal way, the efficiency of transport for incoherent evolution becomes more better than the coherent one, as sketched in Fig. 6(a). This is an evidence for the preference of the optimal incoherent transport to the coherent one when they are accompanied by this type of harmonic deformations. The oscillations of site 2 and 3 (or 1 and 4) with the same phase, i.e. $\Delta\varphi = 0$, which give the $\zeta_1(t) = \zeta_2(t)$ (see Fig. 7(b)), do not lead to the improvement of incoherent transport relative to the coherent one ,as shown in Fig. 7(a), so it is in agreement with the result of [18].

4 Conclusions

In this paper, we investigated the accompaniment of harmonic deformations, which may be created from thermal fluctuations, with the optimal coherent and incoherent quantum transport. For the configurations discussed in this paper, and for many similar but complex ones, in the absence of deformations, the optimal transport is only the pure coherent transport. However, we found out that, in the presence of some rare harmonic deformations, optimal transport is pure incoherent one. This, indeed, induces the notion in mind that the environmental effects on the quantum transport in many body quantum systems may be more efficient than the intrinsic quantum mechanical effects in that systems. The other point, which may be interested in this regard, is the analysis of structural effects of the environments interact with the second configuration via sites 2 and 3, which can be investigated in future.

References

[1] M. B. Plenio, J. Hartley, and J. Eisert, New J. Phys. 6, 36 (2004).

[2] P. J. Pemberton-Ross, and Alastair Kay, Phys. Rev. Leet. 106 (2011) 020503.

[3] V. karimipour, M. Sarmadi Rad, and M. Asoudeh, Phys. Rev. A 85 (2012) 010302(R).

[4] N. Behzadi, S. Kazemi Rudsary, B. Ahansaz Salmasi, Eur. Phys J. D——(2013).

[5] M. Mohseni, P. Rebentrost, S. Lloyd and A. Aspuru-Guzik, J. Chem. Phys. 129, 174106 (2008).

[6] R.J. Sension, Nature 446, 740 (2007).

[7] M. B. Plenio and S. F. Huelga. New J. Phys. 10, 113019 (2008).

[8] F. Caruso, A. W. Chin, A. Datta, S. F. Huelga, and M. B. Plenio, J. Chem. Phys. 131, 105106 (2009).

[9] A. W. Chin, A. Datta, F. Caruso, S. F. Huelga, and M. B. Plenio, New J. Phys. 12, 065002 (2010).

[10] P. Rebentrost, M. Mohseni, I. Kassal, S. Lloyd and A. Aspuru-Guzik, New J. Phys. 11, 0330 (2009).

[11] I. Kassal and A. Aspuru-Guzik, New J. Phys. 14, 053041 (2012).

[12] I. Sinayskiy, A. Marais, F. Petruccione and A. Ekert, Phys. ev. Lett. 108, 020602 (2012).

[13] J. Lim, M. Tame, K. H. Yee, J-S. Lee and J. Lee, New J. Phys. 16, 053018 (2014).

[14] E. J. OReilly and A. Olaya-Castro, Nature Communications,——-, (2014).

[15] E. K. Irish, R. Gomez-Bombarelli and B. W. Lovett, Phys. Rev. A 90, 012510 (2014).

[16] F. L. Semi, K. Furuya and G. J. Milburn, New J. Phys. 12, 083033 (2010).

[17] A. Asadian, M. Tiersch, G. G. Guerreschi, J. Cai, S. Popescu and H. J. Briegel, New J. Phys. 12, 075019 (2010).

[18] F. Caruso, New J. Phys. 16 (2014) 055015

[19] B. Cui, X. X. Yi and C. H. Oh, J. Phys. B: At. Mol. Opt. Phys. 45, 085501 (2012).

[20] N. Behzadi, B. Ahansaz and H. kasani, Phys. Rev. E, ——-, (2015).

[21] M. Christandl, N. Datta, T. C. Dorlas, A. Ekert, A. Kay, and A. J. Landahl, Phys. Rev. A, 71, 032312 (2005).

[22] E. M. Laine, J. Piilo and H. P. Breuer, Phys. Rev. A, 81, 062115 (2010).

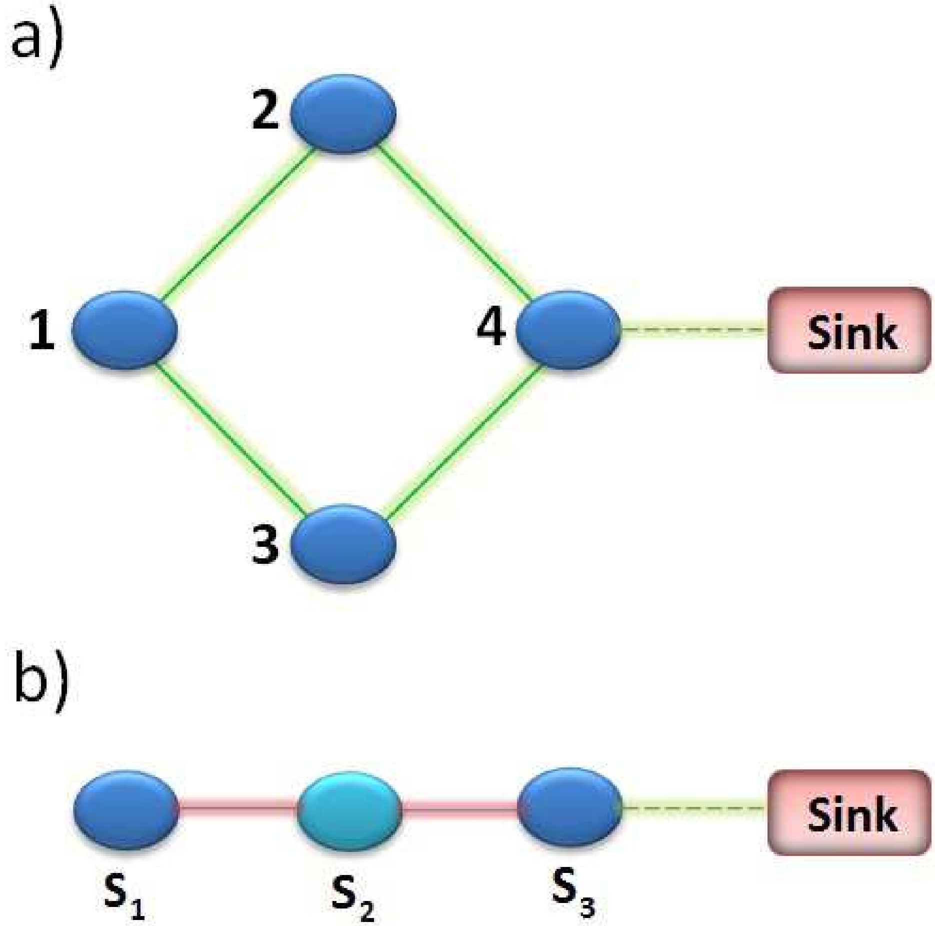

Figure 1:

Fig. 1. (a) Configuration of four interacting two-level atoms with $J_{1,2} = J_{1,3} = J_{2,4} = J_{3,4} = J$, irreversibly connected to the sink site. (b) The equivalent configuration when the set of basis introduced in Eqs. 2, is used.

Fig. 2. (a) Configuration of four interacting two-level atoms with $J_{1,2} = J_{1,3} = J_{2,4} = -J_{3,4} = J$, irreversibly connected to the sink site. Dephasing Markovian noises affect the system through site 2 and 3. (b) The equivalent configuration when the set of basis introduced in Eqs. 4, is used. Invariant subspaces are connected incoherently to each other by the dephasing noises.

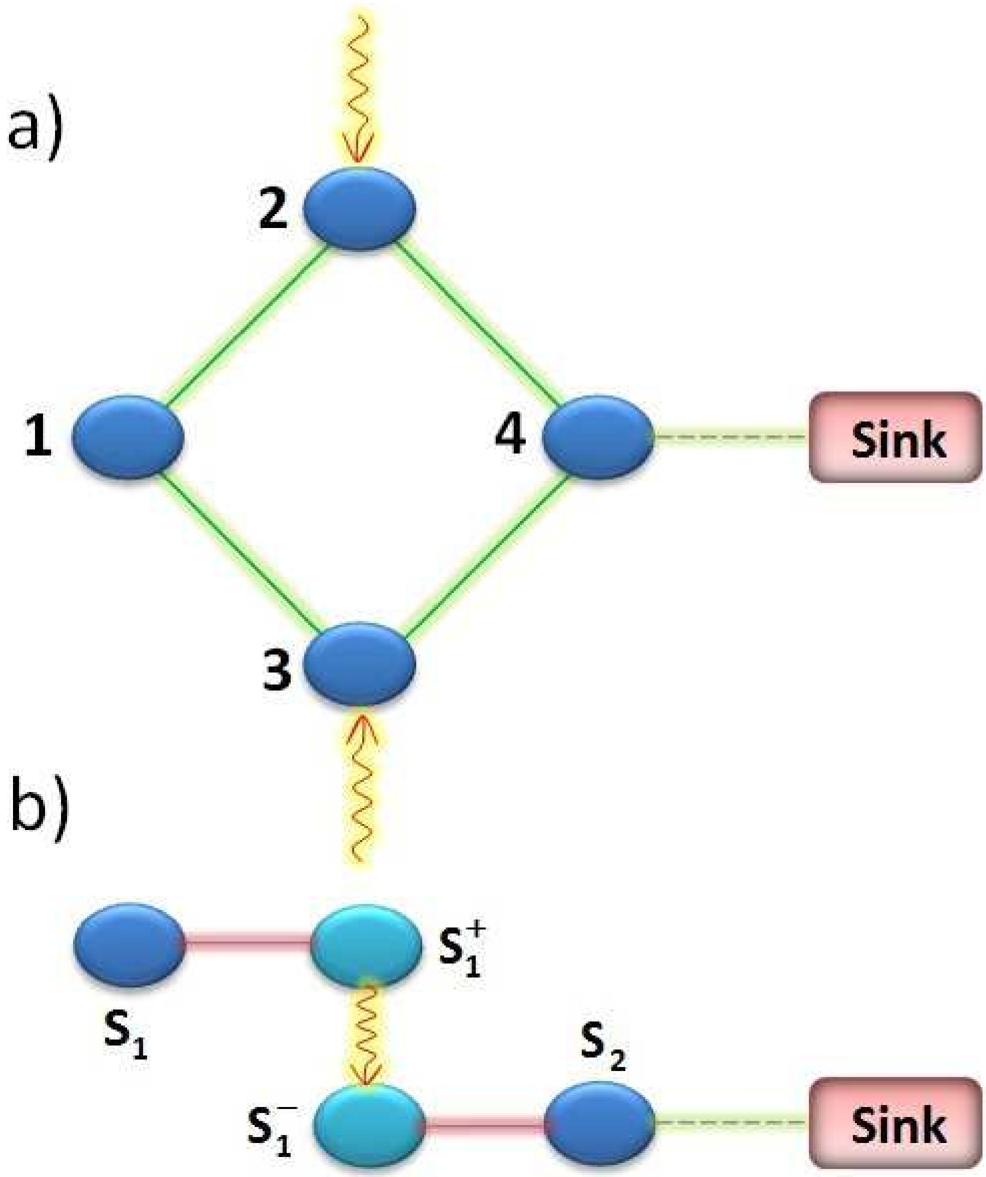

Figure 2:

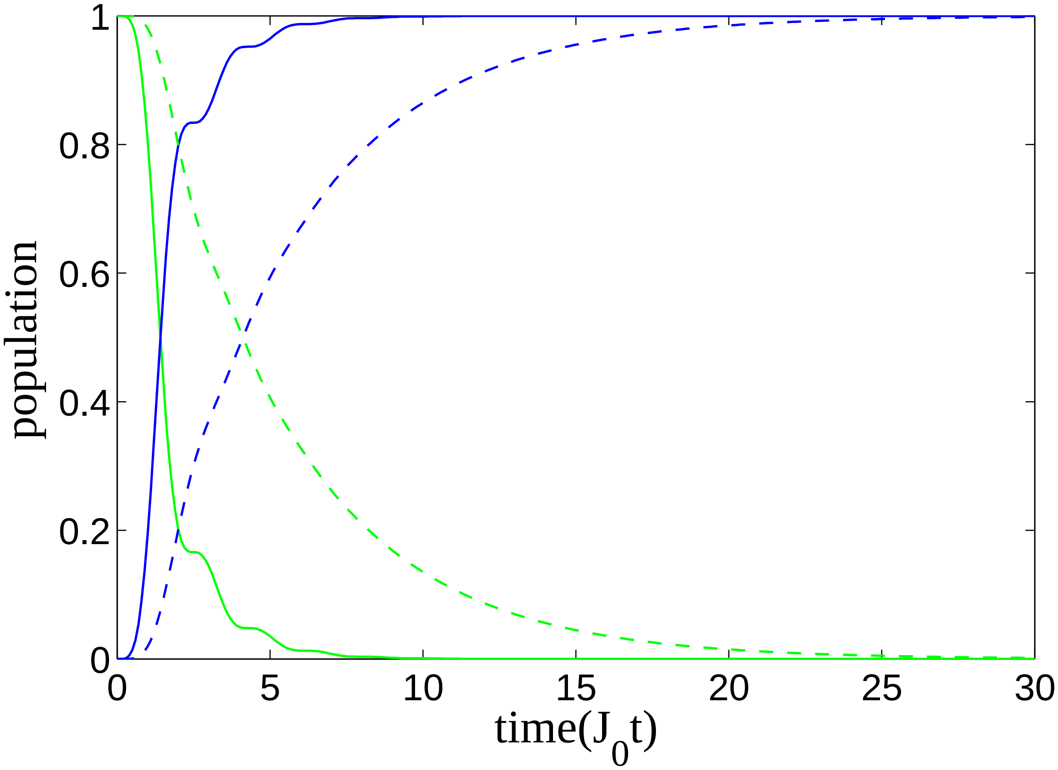

Figure 3:

Fig. 3. The solid and dashed blue curves show the populations of the sinks or optimal efficiency of transports for the coherent and incoherent transfer of excitation through first and second configurations represented in Fig. 1 and Fig. 2 respectively, when all of the sites are fixed. The solid and the dashed green curves indicate the sum of populations of all sites, for the first and second configurations respectively.

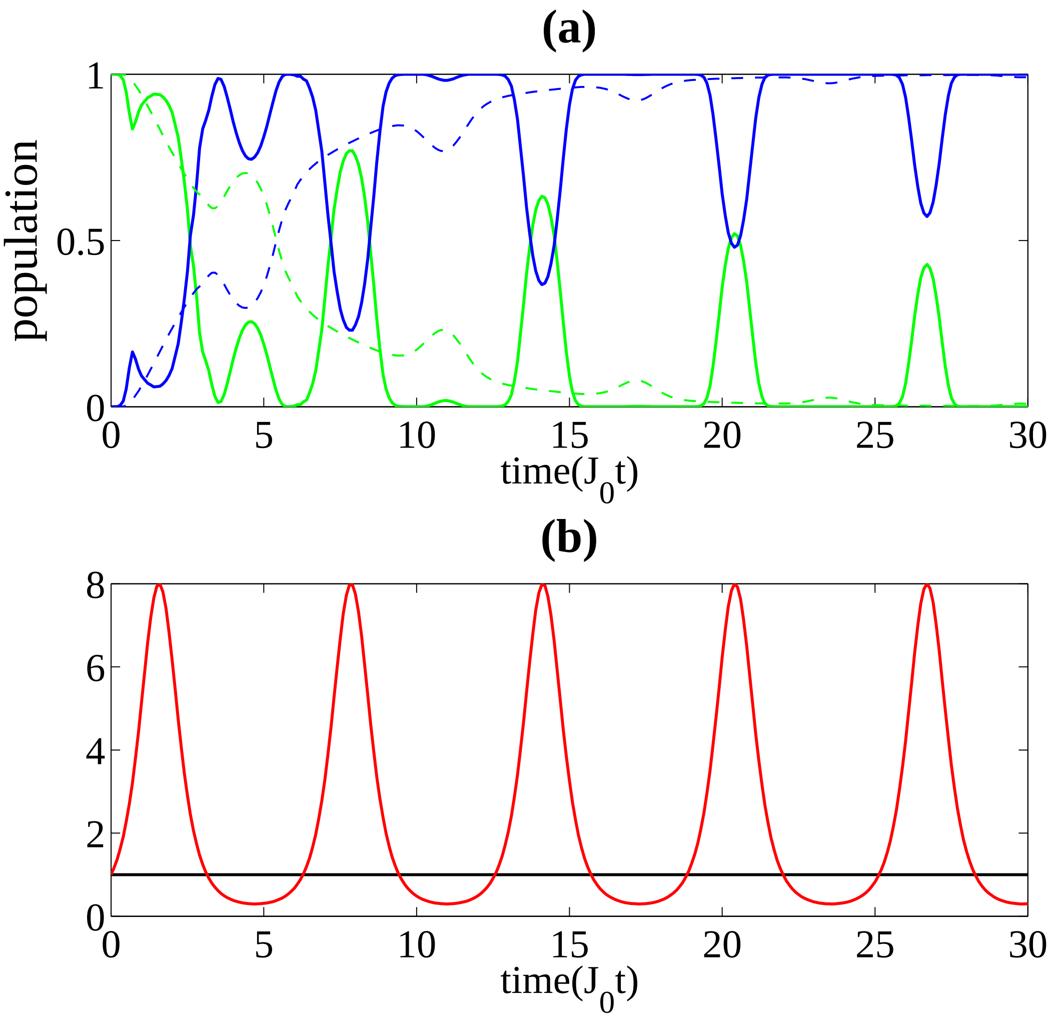

Figure 4:

Fig. 4. (a) Populations of the sinks for the optimal coherent (solid blue curve) and optimal incoherent (dashed blue curve) transport when the site 1 oscillates around its equilibrium along the horizontal line for both configurations with assumptions that, $a = 1/4$, $\phi = 0$ and $\omega_0 = 1$. (b) Time dependent of the coupling strength $\zeta_1(t) = J_{1,2}(t) = J_{1,3}(t)$ (red curve) and $\zeta_2(t) = J_{2,4}(t) = \pm J_{3,4}(t) = 1$ (black curve) where, plus and minus are corresponding to the coherent and incoherent transports respectively.

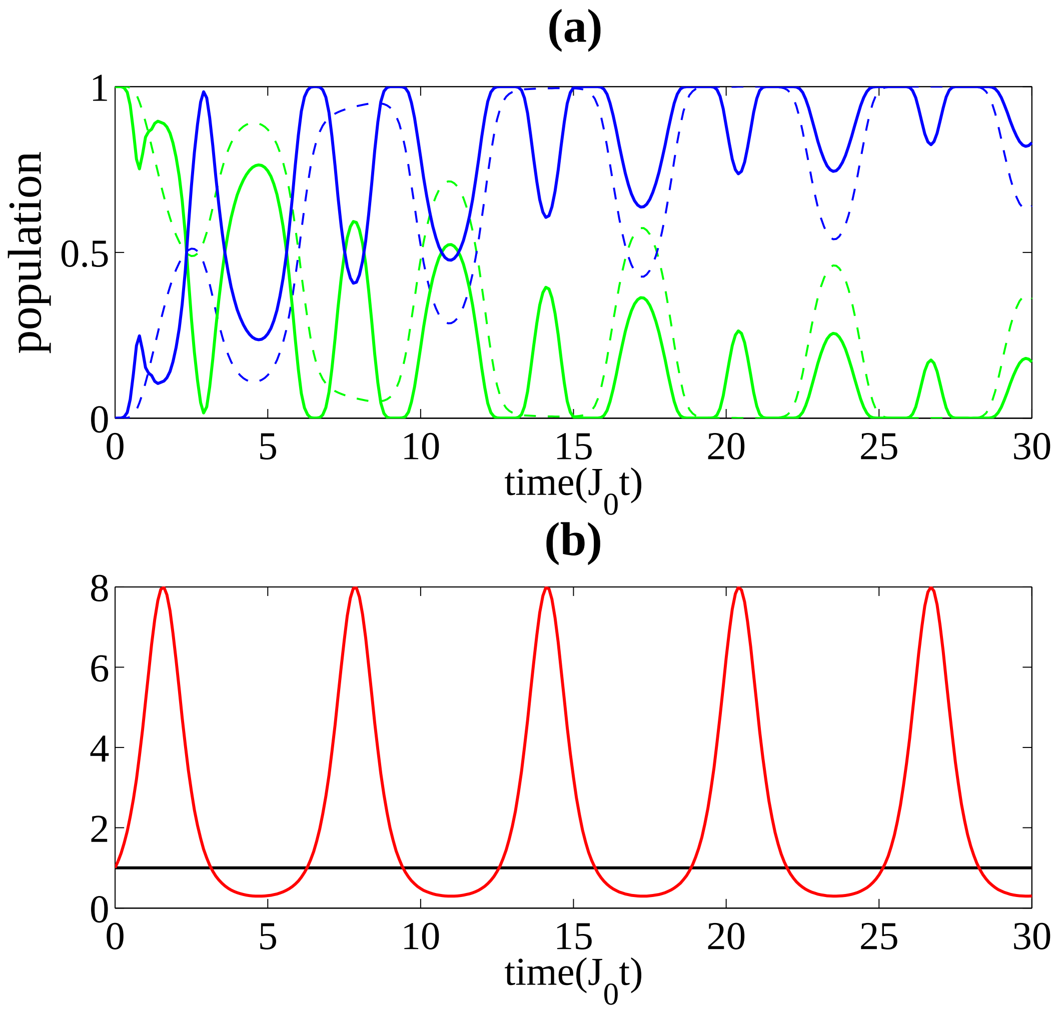

Figure 5:

Fig. 5. (a) Populations of the sinks for the optimal coherent (solid blue curve) and optimal incoherent (dashed blue curve) transport when the site 4 oscillates around its equilibrium along the horizontal line for both configurations with assumptions that, $a = 1/4$, $\phi = 0$ and $\omega_0 = 1$. (b) Time dependent of the coupling strength $\zeta_1(t) = J_{1,2}(t) = J_{1,3}(t) = 1$ (black curve) and $\zeta_2(t) = J_{2,4}(t) = \pm J_{3,4}(t)$ (red curve).

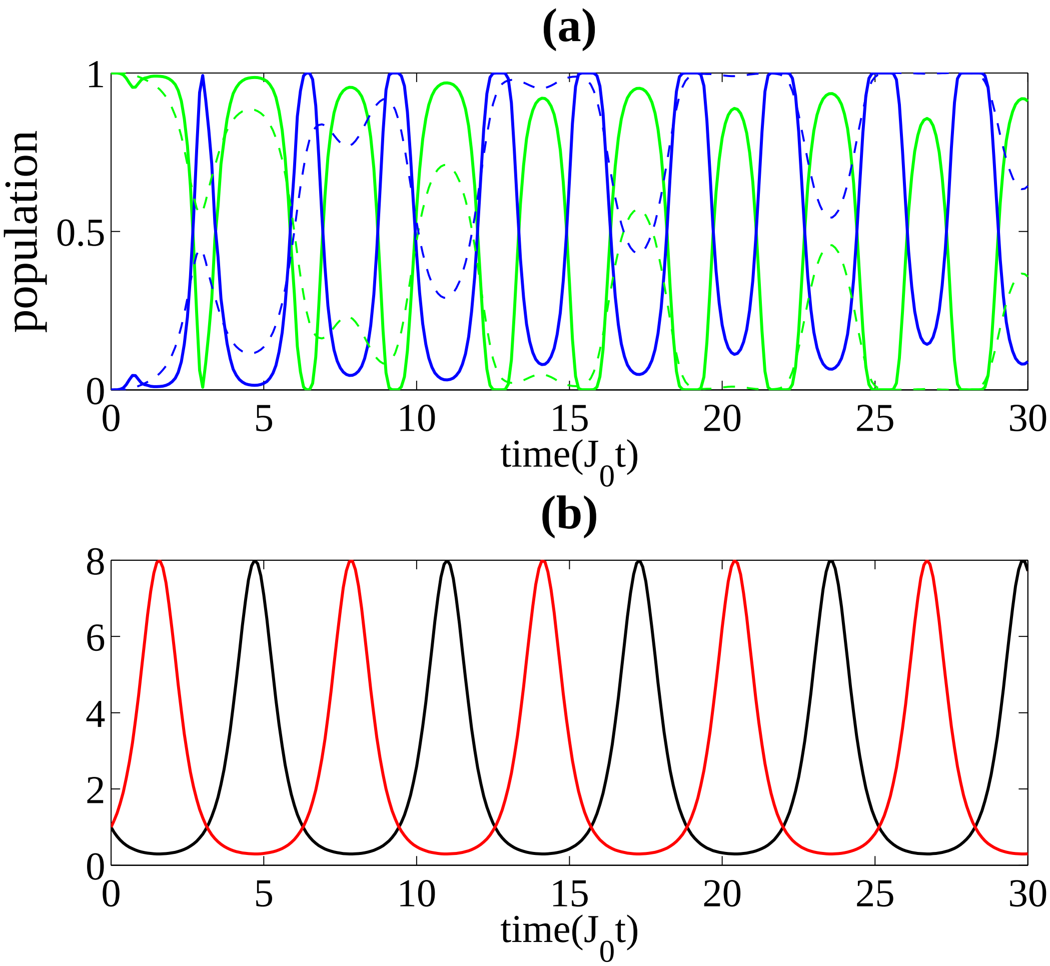

Figure 6:

Fig. 6. (a) Populations of the sinks for the optimal coherent (solid blue curve) and optimal incoherent (dashed blue curve) transport when the sites 1 and 4 oscillate around their equilibrium positions with the phase difference $\Delta\phi = \pi$, along the horizontal line with assumptions for each of the oscillations that, $a = 1/4$ and $\omega_0 = 1$. (b) Time dependent of the coupling strength $\zeta_1(t) = J_{1,2}(t) = J_{1,3}(t)$ (black curve) and $\zeta_2(t) = J_{2,4}(t) = \pm J_{3,4}(t)$ (red curve).

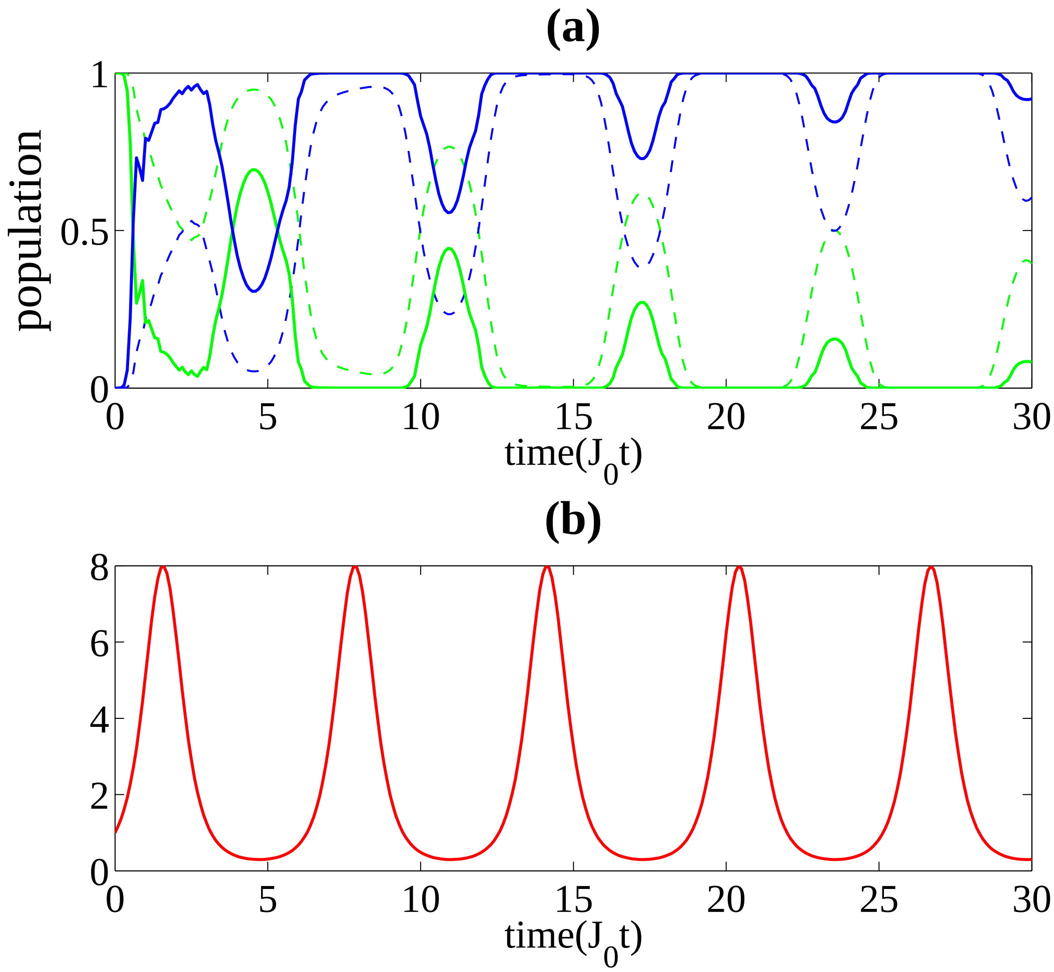

Figure 7:

Fig. 7. (a) Populations of the sinks for the optimal coherent (solid blue curve) and optimal incoherent (dashed blue curve) transport when the sites 2 and 3 (or site1 and 4) oscillate around their equilibrium positions with the phase difference $\Delta\phi = 0$, along the vertical line (horizontal line) with assumptions for each of the oscillations that, $a = 1/4$ and $\omega_0 = 1$. (b) Time dependent of the coupling strength $\zeta_1(t) = J_{1,2}(t) = J_{1,3}(t) = \zeta_2(t) = J_{2,4}(t) = \pm J_{3,4}(t)$.