Global coherence of quantum evolutions based on decoherent histories: theory and application to photosynthetic quantum energy transport

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Abstract

In this paper we address the problem of characterizing coherence in dissipative (Markovian) quantum evolutions. We base our analysis on the decoherent histories formalism which is the most basic and proper approach to assess coherence properties of quantum evolutions. We introduce and test different quantifiers and we show how these are able to capture the (average) coherence of general quantum evolutions on various time scales and for different levels of environmentally induced decoherence. In order to show the effectiveness of the introduced tools, we thoroughly apply them to a paradigmatic instance of quantum process where the role of coherence is being hotly debated: exciton transport in the FMO photosynthetic complex and its most relevant trimeric subunit. Our analysis illustrates how the high efficiency of environmentally assisted transport can be traced back to the coherence properties of the evolution and the interference between pathways in the decoherent histories formalism. Indeed, we show that the bath essentially implements a quantum recoil avoiding effect on the exciton dynamics: the action of decoherence in the system is set at precisely the right level needed to preserve and sustain the benefits of the fast initial quantum delocalization of the exciton over the network, while preventing the subsequent recoil that would necessarily follow from a purely coherent dynamics. This picture becomes very clear when expressed in terms of pathways leading to the exit site: the action of the bath is seen to selectively kill the negative interference between pathways, while retaining the initial positive one.
I. INTRODUCTION

Transport processes at the nanoscale are an arduous challenge to the quantum physicist. When seeking for a detailed understanding of these complex phenomena, which is essential for applications to energy and information transfer, we are bound to move along the border between quantum and classical physics. While classical models of transport clearly break down at the nanoscale, purely quantum, coherent models are equally unfit to provide a satisfactory description, because the systems of interest are strongly coupled to their surroundings. One has therefore to enlarge one’s vision and develop kinetic models involving coherent as well as incoherent terms. In this realm, the usual picture of ‘noise’ would be quite misleading to depict the effects of the environment, as the latter plays a critical role in the transport process, altering the transport properties to a nonperturbative, qualitative extent.

There is now an emerging consensus that efficient transport builds on a finely tuned balance of quantum coherence and decoherence caused by environmental noise [12], a phenomenon known as environmentally assisted quantum transport (ENAQT). This paradigm has emerged with clarity in recent years, as growth of interest in quantum transport models was fueled by the study of energy transfer in light-harvesting systems. Since modern spectroscopic techniques first suggested that exciton transport within photosynthetic complexes might be coherent over appreciable timescales [2], a growing number of experiments has provided solid evidence that coherent dynamics occurs even at room temperature for unusually long timescales (of the order of 100 fs) [3, 4]. Efforts to model these systems have led to general models of ENAQT [5–7], depicting the complex interplay of three key factors: coherent motion through quantum delocalization, environmental decoherence, and localization caused by a disordered energy landscape.

So far, the presence of coherence in light-harvesting systems has been qualitatively associated to the observation of distinctive ‘quantum features’. Originally, coherence was identified with ‘quantum wavelike’ behavior as reflected by quantum beats in the dynamics of chromophore populations within a photosynthetic complex. Later works, employing quantum-information concepts and techniques, have switched attention towards quantum correlations between chromophores, in particular quantum entanglement. Besides being open to criticism (see, e.g., [19, 20]), these approaches do not provide a quantitative and universal definition of coherence.

In this work, we take a different perspective and we address coherence in what is a very general and appropriate framework. To do so we choose to resort to the most fundamental manifestation of
coherence – quantum interference. A completely general and fundamental formalism to describe quantum interference is provided by the decoherent histories (DH) approach to quantum mechanics. DH have mainly served to deal with foundational issues of quantum mechanics - such as providing a consistent framework to describe closed quantum systems or elucidate the emergence of classical mechanics from a quantum substrate. However, DH can also be a valid and systematic tool in quantifying interference in quantum processes, and discussing its relevance therein. Indeed, DH provide a precise mathematical formalization of interference by means of the the so called decoherence matrix $\mathcal{D}$. The latter is built on the elementary notion of histories and allows one to describe the quantum features vs the classical ones in terms of interference between histories, or pathways if one resorts to the mental picture of the double slit experiments. It is however difficult to quantify in a compact and meaningful way the content of $\mathcal{D}$ and its implications for the dynamics of specific systems. Our main goal is therefore twofold: on one hand we define a functional $C$ that allows one to express the coherence content of a general quantum evolution at its various time scales; on other hand we show that the judicious combination of $C$ and functions of sub-blocks of $\mathcal{D}$ constitute the natural way to investigate coherence in quantum transport phenomena, where excitons move along different pathways that mutually interfere, constructively or destructively, and therefore delocalize over the transport network.

In what follows, we shall investigate DH for a simple yet fundamental model of quantum energy transfer: the FMO (refs.) and in particular a relevant trimeric subunit. For simplicity, we will use the well-known Haken-Strobl model [8] to describe Hamiltonian and dephasing dynamics. We shall initially focus on our new coherence measure $C$, characterize its behaviour and verify that it can consistently identify the bases and timescales over which quantum coherent phenomena are present during the evolution of the system. We then identify the proper time scale over which quantum delocalization takes place and show how the average coherence exhibited on those time scales can be connected with the delocalization process. A more detailed analysis will be aimed at distinguishing between constructive and destructive interference affecting the histories ending at the site where the excitation exits the photosynthetic structure. By using again the decoherence functional, we will show that the beneficial role of dephasing for the transport efficiency lies in a selective suppression of destructive interference, something that was systematically suggested but never expressed within a rigorous framework.

While our main goal is to discuss energy transfer in complete photosynthetic complexes, we prefer to look at a simpler system first, which will allow to single out more clearly relevant features that
also appear in more complex systems. We will thus begin by considering a trimer, that is virtually
the simplest paradigmatic model retaining the basic characteristics of a disordered transfer network
and it can also be conceived as an essential building block of a larger network. Upon analyzing
the trimer, we will be able to repeat the basis lines of argument for a more complex systems such
as the photosynthetic unit FMO.

II. DECOHERENT HISTORIES

The formalism of decoherent (or consistent) histories was developed in slightly different flavors
by Griffiths [21], Omnès [23], Hartle and Gell-Mann [24]. DH provide a consistent formulation of
quantum mechanics where probabilities of measurement outcomes are replaced by probabilities of
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The idea of ‘histories’ stems from Feynman’s ‘sum-over-histories’ formulation of quantum me-

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theory and gives a prescription to attribute probabilities to (sets of) histories. A history is defined
as a sequence of projectors at times $t_1 \ldots t_N$ we get

$$
\langle \psi_f | U(t_f - t_0) | \psi_i \rangle = \sum_{j_1} \sum_{j_N} \langle \psi_f | P_{j_N} U(t_N - t_{N-1}) \ldots U(t_2 - t_1) \sum_{j_1} P_{j_1} U(t_1 - t_0) | \psi_i \rangle
$$

where we use the Heisenberg notation $P_j(t) = U^\dagger(t - t_0) P_j U(t - t_0)$. Thus the total amplitude

$$
\langle \psi_f | U(t_f - t_0) | \psi_i \rangle
$$

is decomposed as a sum of amplitudes, each one corresponding to a different

history identified by a sequence of projectors $P_{j_N} \ldots P_{j_1}$.

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theory and gives a prescription to attribute probabilities to (sets of) histories. A history is defined
as a sequence of projectors at times $t_1 < \cdots < t_N$. Probabilities can be assigned within exhaustive
sets of exclusive histories, i.e., sets of histories $S_N = \{t_1, \ldots, t_N, P_{j_1}, \ldots, P_{j_N}\}$ where subscripts

$\{j_1, \ldots, j_N\}$ label different alternatives at times $t_1, \ldots, t_N$. Histories are exhaustive and exclusive.
in the sense that the projectors at each time satisfy relations of orthogonality \( P_j P_k = \delta_{jk} P_j \), and completeness, \( \sum_j P_j = \mathbb{I} \). In other words, the projectors \( P_j \) define a projective measurement. Within a specified set, any history can be identified with the sequence of alternatives \( j \equiv j_1, \ldots, j_N \) realized at times \( t_1, \ldots, t_N \).

Different alternative histories can be grouped together with a procedure called *coarse-graining*. Starting from histories \( j \) and \( k \) we can define a new, *coarse-grained* history \( m = j \lor k \) by summing projectors for all times \( t_\ell \) such that \( j_\ell \) and \( k_\ell \) differ:

\[
P_{m_\ell} = P_{j_\ell} + P_{k_\ell} \text{ if } j_\ell \neq k_\ell, \\
P_{m_\ell} = P_{j_\ell} \text{ if } j_\ell = k_\ell,
\]

for all \( \ell = 1, \ldots, N \). By iterating this procedure, one can obtain more and more coarse-grained histories. A special type of coarse-graining is the *temporal coarse-graining*: we group together histories \( j, k, \ldots, l \) such that at some time \( t_\ell \) we have \( P_{j_\ell} + \ldots P_{k_\ell} + \ldots P_{l_\ell} = \mathbb{I} \). Then the coarse-grained history \( m = j \lor k \lor \ldots \lor l \) contains only one-projector (equal to the identity) at time \( t_\ell \), that can be neglected and hence removed from the string of projectors defining the history.

On the other hand *temporal fine-graining* can be implemented for example by allowing different alternatives at a times \( t_k \not\in \{t_1, \ldots, t_N\} \). In particular one can create new sets of histories \( S_{N+1} = \{t_1, \ldots, t_N, t_{N+1}, P_{j_1}, \ldots, P_{j_N}, P_{j_{N+1}}\} \) from a given one \( S_N \) by adding different alternatives at time \( t_{N+1} > t_N \); \( S_{N+1} \) are fine grained versions of the sets \( S_N \).

Once we specify the initial state \( \rho \) and the (unitary) time evolution \( U(t) \), we can assign any history \( j \) a weight

\[
w_j = \text{Tr}[C_j \rho C_j^\dagger], \quad \text{with} \quad C_j = P_{j_N}(t_N) \ldots P_{j_1}(t_1)
\]

where we use the Heisenberg notation \( P_{j_\ell}(t_\ell) = U(t_\ell)P_{j_\ell}U(t_\ell)^\dagger \). When the initial state is pure, \( \rho = |\psi_i\rangle \langle \psi_i| \) and the final projectors are one dimensional, \( P_{j_N} = |\psi_{j_N}\rangle \langle \psi_{j_N}| \), this formula takes the simple form of a squared amplitude

\[
w_j = |\langle \psi_{j_N}|P_{j_{N-1}}(t_{N-1}) \ldots P_{j_1}(t_1)|\psi_i\rangle|^2
\]

Weights cannot be interpreted as true probabilities, in general. Indeed, due to quantum interference between histories, the \( w_j \) do not behave as classical probabilities. Indeed, consider two exclusive histories \( j, k \in S \) and the relative coarse-grained history \( m = j \lor k \) by: \( P_{m_\ell} = P_{j_\ell} + P_{k_\ell}, \forall \ell \). If the \( w_j \) were real probabilities, we would expect \( w_m = w_j + w_k \). Instead, what we find is

\[
w_m = w_j + w_k + 2 \text{Re}(\text{Tr}[C_j \rho C_k^\dagger])
\]
Due to the non-classical term $Re(\text{Tr}[C_j \rho C_k^\dagger])$, representing quantum interference between the histories $j$ and $k$, the classical probability-sum-rule is violated. The matrix

$$D_{jk} = \text{Tr}[C_j \rho C_k^\dagger] = \text{Tr}[P_{jN} U(t_N - t_{N-1}) \ldots P_{j1} U(t_1) \rho U(t_1)^\dagger P_{k1} \ldots U(t_N - t_{N-1})^\dagger P_{kN}]$$

(2)

is called decoherence matrix. Its diagonal elements are the weights of histories and its off-diagonal elements are interferences between pairs of histories. The decoherence matrix has the following properties: i) it is Hermitian ii) it is semipositive definite iii) it is trace one iv) it is block-diagonal in the last index, $D_{jk} = \delta_{jNkN} D_{jk}$. Weights of coarse-grained histories can be obtained by summing matrix entries in an $n \times n$ block of the decoherence matrix corresponding to the original fine-grained histories. For instance, the weight of history $m = j \lor k$ is obtained by summing entries of a $2 \times 2$ block of the decoherence matrix,

$$w_m = D_{jj} + D_{kk} + D_{jk} + D_{kj}$$

A necessary and sufficient condition to guarantee that the probability sum rule $w_{j \lor k} = w_j + w_k$ apply within a set of histories is

$$Re[D_{jk}] = 0, \forall j \neq k.$$

This condition is termed as weak decoherence; the necessary and sufficient condition that is typically satisfied and that we will adopt in the following is the stronger one termed as medium decoherence

$$D_{jk} = 0, \forall j \neq k.$$  

(3)

Medium decoherence implies weak decoherence. Any exhaustive and set of exclusive histories satisfying medium decoherence is called a decoherent set. The fundamental rule of DH approach is that probabilities can be assigned within a decoherent set, each history being assigned a probability equal to its weight. If medium decoherence holds, the diagonal elements of the decoherence matrix can be identified as real probabilities for histories and we can write $D_{jj} = p_j$.

Due to property iv), if we perform a temporal coarse-graining over all times except the last, we obtain ‘histories’ with only one projection, $P_{jN}$ at the final time $t_N$. These histories automatically satisfy medium decoherence:

$$\sum_{j_1, \ldots, j_{N-1}} \sum_{k_1, \ldots, k_{N-1}} D_{jk} = \delta_{jNkN} \text{Tr}[P_{jN} (t_N) \rho P_{jN} (t_N)] \equiv \delta_{jNkN} p_{jN}$$
where \( p_{jN} \equiv \text{Tr}[P_{jN}(t_N) \rho P_{jN}(t_N)] \) is the probability that the system is in \( j_N \) at time \( t_N \). Due to interference, the probability of being in \( j_N \) at time \( t_N \) is not simply the sum of probabilities of all alternative paths leading to \( j_N \), i.e., of all alternative histories with final projection \( P_{jN} \). In formulas,

\[
p_{jN} \neq \sum_{j_1,..,j_{N-1}} w_j = \sum_{j_1,..,j_{N-1}} D_{jj}
\]

The probability and global interference of histories \( \mathcal{I}_{jN}(\tau) \) ending in \( j_N \) can be thus expressed as

\[
p_{jN}(\tau) = \sum_{j_1,..,j_{N-1}} w_j(\tau) + \mathcal{I}_{jN}(\tau)
\]

with \( \tau = N \Delta t \). Destructive interference will happen when \( \mathcal{I}_{jN} < 0 \), constructive interference when \( \mathcal{I}_{jN} > 0 \).

Given a factorization of the Hilbert space into a subsystem of interest and the rest (environment), \( \mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_E \), the events of a history take the form \( P_{j_t j_{t'}^e} = \tilde{P}_{j_t} \otimes \Pi_{j_{t'}^e} \) where \( \tilde{P}_{j_t} \) and \( \Pi_{j_{t'}^e} \) are projectors onto Hilbert subspaces of \( \mathcal{H}_S \) and \( \mathcal{H}_E \) respectively. Histories for \( S \) alone can be obtained upon considering appropriate coarse-grainings over the environment degrees of freedom, such that the events are \( \tilde{P}_{j_t} \otimes I_E \) where \( I_E \) is the identity over \( \mathcal{H}_E \). Upon introducing the time-evolution propagator \( \mathcal{K}_{t_{t_0}} \) as \( \rho(t) = U(t - t_0) \rho(t_0) U(t - t_0)^\dagger \equiv K_{t_{t_0}}[\rho(t_0)] \) we can rewrite the decoherence matrix as:

\[
D_{jk} = \text{Tr}[\tilde{P}_{jN} \mathcal{K}_{t_{N-1}} \ldots \mathcal{K}_{t_{N_0}} \tilde{P}_{kN}] \quad \mathcal{K}_{t_{t_0}}[\rho(t_0)]
\]

If the initial state is factorized \( \rho(t_0) = \tilde{\rho}_S(t_0) \otimes \rho_E(t_0) \), then the reduced density matrix \( \rho_S(t) = \text{Tr}_E[\rho(t)] \) evolves according to \( \tilde{\rho}_S(t) = K_{t_{t_0}} \tilde{\rho}_S(t_0) \) where \( \tilde{K} \) is the (non-unitary) reduced propagator defined by

\[
\text{Tr}_E[U(t - t_0) \tilde{\rho}_S(t_0) \otimes \rho_E(t_0) U^\dagger(t - t_0)] = \tilde{K}_{t_{t_0}}[\tilde{\rho}_S(t_0)]
\]

If the evolution of the system and environment is Markovian, we can write \( \tilde{K}_{t_{t'}} = \tilde{K}_{t_{t'-t'}} \).

As proved by Zurek [25], under the assumption of Markovianity we can rewrite the decoherence matrix in terms of reduced quantities alone, i.e., quantities pertaining to the system only:

\[
D_{jk} = \text{Tr}_S[\tilde{P}_{jN} \tilde{K}_{t_{N-1}} \ldots \tilde{K}_{t_{N_0}} \tilde{P}_{kN}] \]

\[
= \text{Tr}_S[\tilde{P}_{jN} \tilde{K}_{t_{N-1}} \ldots \tilde{K}_{t_{N_0}} \tilde{P}_{kN}] 
\]
III. THE COHERENCE MEASURE $C$

The DH approach provides the most fundamental framework in which the transition from quantum to classical realm can be expressed. Indeed, it is based on the most basic feature that characterize the quantum world: interference and the resulting coherence of dynamical evolution. Despite being a well developed field of study, the DH history approach lacks of a proper global measure of the coherence produced by the dynamics at the different time scales. We therefore introduce a quantifier that measures the global amount of coherence within a set of histories. Assume projectors for all times $t_{\ell}, \ell = 1, \ldots, N$ are taken in a fixed basis $|e_j\rangle$, $P_{j} = |e_j\rangle\langle e_j|$. Assume further that histories are composed by taking equally spaced times between consecutive measurements i.e., $t_1 = \Delta t, \ldots, t_N = N\Delta t$. (in other words, histories correspond to the measurement applied in the same basis and repeated at regular times). For such a set of histories, consider the decoherence matrix

$$D_{jk}^{(N,P,\Delta t)} = \text{Tr}[C_{j}^{(N,P,\Delta t)} \varrho C_{k}^{(N,P,\Delta t)}]$$

where $C_{j}^{(N,P,\Delta t)} = P_{j,N} (N\Delta t) \ldots P_{j,1} (\Delta t)$. Take the von Neumann entropy of the decoherence matrix,

$$h(P, N, \Delta t) = -\text{Tr}[D^{(N,P,\Delta t)} \log D^{(N,P,\Delta t)}]$$

Due to coherence between histories, $h_N$ differs from the ‘classical-like’ Shannon entropy of history weights

$$h^{(c)}(P, N, \Delta t) = -\sum_{j} w_{j}^{(N,P,\Delta t)} \log w_{j}^{(N,P,\Delta t)}$$

where $w_{j}^{(N,P,\Delta t)} = \text{Tr}[C_{j}^{(N,P,\Delta t)} \varrho C_{j}^{(N,P,\Delta t)}]$ are the diagonal elements of $D^{(N,P,\Delta t)}$ i.e., the weights. The difference between the two quantities is wider if off-diagonal elements of the decoherence matrix are bigger, i.e., if the set of histories is more coherent. Let us define:

$$C(P, N, \Delta t) \equiv \frac{h^{(c)}(P, N, \Delta t) - h(P, N, \Delta t)}{h^{(c)}(P, N, \Delta t)}$$

We argue that $C(P, N, \Delta t)$ is suitable to be used as a general measure of coherence within the set of histories defined by $P, N, \Delta t$. Indeed, we can readily prove the following properties:

- i) $0 \leq C(P, N, \Delta t) < 1$. To prove $C(P, N, \Delta t) > 0$, let us define a matrix $\tilde{D}_{jk}^{(N,P,\Delta t)} = \delta_{jk} D_{jk}^{(N,P,\Delta t)}$ where the off-diagonal entries are set to zero. Since

$$\text{Tr}[D^{(N)} \log \tilde{D}^{(N)}] = \sum_j D_{jj}^{(N,P,\Delta t)} \log D_{jj}^{(N,P,\Delta t)} = \text{Tr}[\tilde{D}^{(N,P,\Delta t)} \log \tilde{D}^{(N,P,\Delta t)}]$$


we obtain that the numerator of \((??)\) can be expressed as a quantum relative entropy:

\[
\begin{align*}
    h^{(c)}(P, N, \Delta t) &- h(P, N, \Delta t) = -\text{Tr}[\tilde{D}^{(N,P,\Delta t)} \log \tilde{D}^{(N,P,\Delta t)}] + \\
    \text{Tr}[D^{(N,P,\Delta t)} \log D^{(N,P,\Delta t)}] &- \text{Tr}[\tilde{D}^{(N,P,\Delta t)} (\log D^{(N,P,\Delta t)} - \log \tilde{D}^{(N,P,\Delta t)})] \\
    &= h(D^{(N,P,\Delta t)} || \tilde{D}^{(N,P,\Delta t)}) \geq 0
\end{align*}
\]

where \(h(A || B) \geq 0\) is the relative entropy between \(A\) and \(B\).

\begin{itemize}
  \item ii) \(C(P, N, \Delta t) = 0\) iff \(D^{(N,P,\Delta t)}_{jj} = \tilde{D}^{(N,P,\Delta t)}_{jj}\), i.e., \(C(P, N, \Delta t)\) vanishes if medium decoherence holds for the set of histories. Since the two quantities, \(h(N, P, \Delta t)\) and \(h^{(c)}(N, P, \Delta t)\) coincide in this case.
\end{itemize}

Thus \(C(P, N, \Delta t)\) is in essence a (statistical) distance between the decoherence matrix \(D\) and the corresponding diagonal matrix \(\tilde{D}^{(P,N,\Delta t)}\), renormalized so that its value lies between 0 and 1. The distance is the greater, the grater are the off-diagonal elements of \(D^{(P,N,\Delta t)}\). The meaning of \(C(P, N, \Delta t)\) can be easily understood if we use linear entropy, a lower bound the logarithmic version,

\[
\begin{align*}
    h_L(P, N, \Delta t) &= 1 - \text{Tr}[(D^{(N,P,\Delta t)})^2], \quad 1 - h^{(c)}_L(P, N, \Delta t) = \text{Tr}[(\tilde{D}^{(N,P,\Delta t)})^2]
\end{align*}
\]

In this case, we obtain a ‘linear entropy’ proxy of \(C(N, P, \Delta t)\) as:

\[
C_L(P, N, \Delta t) \equiv \frac{h^{(c)}_L(P, N, \Delta t) - h_L(P, N, \Delta t)}{h^{(c)}_L(P, N, \Delta t)} = \frac{\sum_{j \neq k} |D^{(N,P,\Delta t)}_{jk}|^2}{1 - \sum_j |D^{(N,P,\Delta t)}_{jj}|^2}
\]

which is a simplified version that, by avoiding the diagonalization of \(D^{(N,P,\Delta t)}\), helps containing the numerical complexity.

The measure introduced is well grounded on physical considerations. In the following we will apply it to a simple system in order to check its consistency and later to use it to charcterized the coherence properties of the evolution induced by various regimes of interaction with the environment. What one has to first check is whether the measure properly takes into account the action of the bath. In particular, if the bath are characterized by a decoherence time \(\gamma^{-1}\), it is known ([25]) that on time scales \(\Delta t \geq \gamma^{-1}\) the decoherent matrix becomes diagonal: the probability of an history at time \(t_{N+1}\) can be fully determined by its probability at time \(t_N\) since no interference can occur between different histories. Indeed, the action of the bath is to create a \textit{decoherent set of histories} that are defined by a proper measurement basis: the pointer basis ([25]). Therefore the
fine graining procedure obtained by constructing a set of histories $S_{N+1}$ via the addition of new complete measurements in the same basis at time $t_{N+1} = (N + 1)\Delta t$ to the set $S_N$, should leave the coherence functional $C$ invariant i.e., $C(P, N + 1, \Delta t) \approx C(P, N, \Delta t)$. If instead $\Delta t < \gamma^{-1}$ the same fine graining procedure should lead to $C(P, N + 1, \Delta t) \geq C(P, N, \Delta t)$.

Before passing to analyze the specific system we want to focus on the complexity of the evaluation of $D$ and $C$. The dimension of the decoherent matrix grows with the dimension $d$ of the basis $P$ and the number $N$ of instant of times that define each history as $d^{2N}$. This exponential growth in principle limits the application of the DH approach to small systems. However, as for the system considered in this paper the computational effort is contained due to the small number of subsystems (chromophores) and the small dimension of the Hilbert space which is limited to the single exciton manifold. As we shall see, by limiting the choice of $N$ to a reasonable number, the analysis can be fruitfully carried even on a laptop.
We now start to analyze decoherent histories in simple models of energy transfer composed of a small number $d$ of chromophores (sites). Neglecting higher excitations, each site $i$ can be in its ground $|0\rangle_i$ or excited $|1\rangle_i$ state. We work in the single excitation manifold, and define the site basis as

$$|i\rangle \equiv |0\rangle_1 \ldots |1\rangle_i \ldots |0\rangle_d \quad i = 1 \ldots d$$

i.e. state $|i\rangle$ represents the exciton localized at site $i$. On-site energies and couplings are represented by a Hamiltonian $H$ that is responsible for the unitary part of the dynamics. Interaction with the environment is implemented by the Haken-Strobl model, that has been extensively used in models of ENAQT [5, 7]. The effect of the environment is represented by a Markovian dephasing in the site basis, expressed by Lindblad terms $L$ in the evolution, as follows:

$$\dot{\rho} = [H, \rho] + \sum_i \gamma_i [2 \rho L_i L_i^\dagger - L_i^\dagger L_i \rho - \rho L_i^\dagger L_i]$$

where $L_i = |i\rangle \langle i|$ are projector onto the site basis, and $\gamma_i$ are the (local) dephasing rates. Furthermore, site $d$ can be incoherently coupled to an exciton sink, represented by a Linblad term,

$$k_{\text{trap}} [2 \rho L_{\text{trap}} L_{\text{trap}}^\dagger - L_{\text{trap}}^\dagger L_{\text{trap}} \rho - \rho L_{\text{trap}}^\dagger L_{\text{trap}}]$$

where $L_{\text{trap}} = |\text{sink}\rangle \langle e|$ and $k_{\text{trap}}$ is the trapping rate. Contrary to other works, we neglect exciton recombination, as it acts on much longer timescales ($1 \text{ ns}$) than dephasing and trapping.

The global evolution is Markovian and it can be represented by means of the Liouville equation

$$\dot{\rho} = \mathcal{L}(\rho) = \mathcal{L}_H(\rho) + \mathcal{L}_\gamma(\rho) + \mathcal{L}_{\text{trap}}(\rho)$$

that can be simply solved by exponentiation,

$$\rho(t) = e^{t\mathcal{L}_t}(\rho(0))$$

In the notation above, the propagator has the form $\tilde{K}_t = e^{t\mathcal{L}(t-t)}$. The efficiency of the transport can be evaluated as the leak of the population $p_e(t) = \langle e|\rho|e \rangle$ of the exit site $e$ towards the sink:

$$\eta(t) = 2k_{\text{trap}} \int_0^t \langle e|\rho|e \rangle$$
the overall efficiency of the process is obtained by letting $t \to \infty$.

While the Markovianity of the model limits the faithful description of decoherence processes actually taking place in real photosynthetic systems, the model retains the basic and commonly accepted aspects of decoherence that acts in site basis: albeit in a complex non-Markovian way, the protein environment measures the system locally i.e., on each site, thus destroying the coherence in site basis and creating it in exciton basis. The model is therefore suitable to readily implement the decoherent histories paradigm and to spot the main basic features we are interested in and that are at the basis of the success of ENAQT.

The FMO unit has 7 chromophores and a complex energy and coupling landscape with no symmetries. Energies and couplings (i.e., the Hamiltonian $H$) can be obtained by different techniques: they can be extracted by means of 2D spectroscopy as in [14] or computed through ab initio calculations as in [15], with similar but not exactly equal results. This very complex structure makes FMO far from ideal as a first example to study. We thus prefer to start by working with a much simpler yet fully relevant subsystem i.e., the trimeric unit composed by the sites 1, 2 and 3 of the FMO complex in the notation of [14, 15]). The first chromophore is the site in which the energy transfer begins, while the third chromophore is the site from which the excitation leaves the complex. The Hamiltonian of the trimeric subunit is [15]

$$H_{Renger} = \begin{pmatrix} 215 & -104.1 & 5.1 \\ -104.1 & 220 & 32.6 \\ 5.1 & 32.6 & 0 \end{pmatrix},$$

(15)

The eigenenergies of the system are given by $E_+ = 322.85 \text{ cm}^{-1}, E_- = 119.13 \text{ cm}^{-1}$, $E_3 = -6.98 \text{ cm}^{-1}$ which corresponds to the eigenfrequencies $f_{ij} = 2\pi\hbar/\Delta E_{ij}$: $f_{+-} = 0.163 \text{ ps}, f_{-3} = 0.100 \text{ ps}, f_{+3} = 0.264 \text{ ps}$. Due its structure, the trimer is a chain composed by a pair of chromophores (1,2), degenerate in energy which form a strongly coupled dimer, and a third chromophore moderately coupled with the second one only. Since in the following we suppose that the exciton starts from site 1, we expect a prominent role of the dimer in the dynamics at least in the first tens of femtoseconds.

In order to show how decoherent histories analysis can be implemented, in the following we will consider histories in site and energy bases $P$ with $N$ measurements at times $n\Delta t$, $n = 1, \ldots, N$. We first use the above introduced coherence function $C(P, N, \Delta t)$ (10) to evaluate the global
coherence of the exciton transport process. In order to test the behaviour of $C$ for different values of dephasing, in Fig. 1, we first plot $C$ as a function of the time interval between measurements for two values of the dephasing rate: 

- $i) \gamma = 0$, corresponding to the full quantum regime (Fig. 1) for the site basis (a);
- $ii) \gamma = 10$ corresponding to an intermediate value of dephasing (Fig. 1) for the site basis (b) and energy basis (c).

Before entering the discussion of the various regimes we note that as a function of the number of measurements $N$ all curves display the expected behaviour: the increase (decrease) of the number of measurements corresponds to a temporal fine graining (coarse graining) of the evolution; therefore, an increase (decrease) of $N$ should imply an increase (decrease) of the amount of coherence between histories. As shown in Fig. (1) the function $C$ correctly reproduces the fine (coarse) graning feature: the qualitative behaviour of $C$ as a function of $\Delta t$ is not affected by the choice of $N$, while an increase of $N$ corresponds, at fixed $\Delta t$, to an increase of $C$.

We will therefore use in the following the value $N = 4$ that allows for a neat description of the phenomena and for a reasonable computational time.

As for the behaviour at fixed $N$ we have that in the full quantum regime ($\gamma = 0$), the system obviously displays coherence in the site basis only since

$$Tr[|E_i\rangle\langle E_i| e^{-iH\Delta t} \rho e^{iH\Delta t} |E_i\rangle\langle E_i|] = \langle E_i|\rho|E_i\rangle \delta_{i,j}$$

and the decoherence matrix $D$ in the energy basis is diagonal and independent on $\Delta t$ and $N$. This simply means that in the pure quantum regime histories in the exciton basis are fully decohered, since the system is not able to create coherence among excitons. Again in the full quantum regime, in site basis, the coherence oscillates as the exciton, starting at site 1 goes back an forth along the trimer, and the evolution builds up coherence in this basis, see Fig. 1 (a). In this regime, the trimer can be approximately seen as a dimer composed by the first two chromophores, and the excitation performs Rabi oscillations with a frequency given by $f_{\pm} = 160 \text{ fs}$; $C$ oscillates at half the frequency: for $\Delta t = 80 \text{ fs}$ the exciton is migrated mostly on site 2 and $C$ has a minimum, which is different from zero since the exciton is partly delocalized on site 3, and the system therefore exhibits a non vanishing coherence.

For intermediate values of $\gamma \approx 10 \text{ ps}^{-1}$, Fig. 1 (b), the coherence in site basis as measured by $C$ correctly drops down at $\Delta t \geq 2\gamma^{-1} [25]$. The dephasing has a strong and obvious effect on the coherence between pathways: coherence in this basis is a monotonic decreasing function of $\gamma$. This is well highlighted by the global coherence function $C$, whose maximal values are reduced
by a factor of $\sim 4$ with respect to those corresponding to full quantum regime. After a time \( \tau_{\text{decoh}} = \gamma^{-1} \) the histories are fully decohered. Indeed, due to the specific model of decoherence (11), which amounts to projective measurements on \( |i\rangle \langle i| \) at each site with a rate \( \gamma \), the system kills the coherence in the site basis, which in turn corresponds to a stable pointer basis for this model [25] i.e., the basis in which the density matrix of the model is forced to be diagonal by the specific decoherence model. On the other hand, see Fig. 1(c), and for the same reason, the dynamics starts to build up coherence in the exciton basis \( |E_i\rangle \langle E_i| \) (which is however later destroyed - on a time scale of approximately 0.2 ps - since the stationary state of the model is the identity. This effect even more evident if one compares the behaviour of \( C \) in exciton basis for different values of \( \gamma \) as shown in Fig. 1(d): \( C \) grows with \( \gamma \) and it lasts over longer time scales. This feature is coherent with the expectations: the equilibrium state for high \( \gamma \) is the identity. Due to the measurements implemented by the environment in site basis, the systems is forced to create coherence in exciton basis. When \( \gamma \) is very high a quantum Zeno effect takes in, the dynamics is blocked, and the time required to reach the equilibrium, and to destroy coherences in all bases, grows consequently.

This first analysis therefore shows that \( C \) is indeed a good candidate for assessing the global coherence properties of quantum evolutions. For fixed number of measurements \( N \), \( C(\Delta t) \) can be interpreted as a measure of the global coherence exhibited by the dynamics over the time scale \( \Delta t \).

We now analyse in detail the specific features of quantum transport for the trimer. The dynamics starts at site 1 and it evolves by delocalizing the exciton on the other chromophores. In order to study this process we first use a measure of delocalization introduced in [11] for the study of LHCII complex dynamics:

\[
\mathcal{H}(t) = - \sum_i p_i(t) \ln p_i(t) 
\]

i.e., the Shannon entropy of \( p_i(t) \), the populations of the three chromophores. This measure allows one to follow how much the exciton gets delocalized over the trimer with time and in different dephasing situations: \( 0 \leq \mathcal{H}(t) \leq \ln(3) \) i.e., \( \mathcal{H} \) is zero when the exciton is localized on a chromophore, and it takes its maximal value when the population of the three sites are equal. In Fig. 2 we plot both \( \mathcal{H}(t) \) and the population \( p_3(t) \) of site 3 for different values of \( \gamma \). Due to the presence of interference, in the mainly quantum regime (\( \gamma = 0.1, \, 1 \text{ ps}^{-1} \)), the exiton first delocalizes mainly over the dimer and partly on the third site: the first maximum corresponds to \( t = 40 \text{ fs} = 4 f_{\perp}^{-1} \) when the system builds up a (close to uniform) coherent superposition between sites 1 and 2, while a non negligible part of the exciton is found in site 3; indeed \( \mathcal{H}(t = 40 \text{ fs}) \approx 0.75 > 0.69 \), the
Figure 1: Coherence function \( C(P, N, \Delta t) \) as a function of \( \Delta t \) for the trimer with Hamiltonian evaluated: in site basis (a), (b) for \( \gamma = 0 \), \( 10 \, ps^{-1} \) and exciton basis (c) for \( \gamma = 10 \, ps^{-1} \); different curves correspond to different numbers of projections \( N = 2, \ldots, 5 \).

Last value corresponding to \( \ln(2) \) i.e., to a uniform superposition over the sites 1 and 2 only. As the dynamics of the systems extends to later times we see that the delocalization \( \mathcal{H}(t) \) and \( p_3(t) \) have an oscillatory behaviour, whose main frequency is \( f_{+-}/2 \), and it approximately corresponds to Rabi oscillations between site 1 and 2, although the initial state fully localized in site 1 cannot be rebuilt due to the presence of site 3. As for the transport, we see that in this regime the system cannot take advantage of the initial fast and high delocalization: the exciton bounces back and forth over the trimer. In the intermediate regime \( \gamma = 16 \, ps^{-1} \), due, as we will later see, to the selective suppression of interference processes, the initial speed up in delocalization is sustained by the dynamical evolution, and the transfer rate to site 3 is correspondingly increased. For very high values of decoherence (\( \gamma = 100 \)) the role of initial interference is suppressed and the initial speed up disappears: the environment measures the system in site basis at high rates and the delocalization process is highly reduced.
The optimal delocalization occurs in correspondence of $\gamma \approx 16 \text{ ps}^{-1}$ and it can be interpolated with a double exponential function

$$H_{\gamma=16}(t) = c_0 + c_1 e^{-t/\tau_1} + c_2 e^{-t/\tau_2}$$

with $c_0 = 1.098 = \ln 3$, $c_1 = -0.84$, $c_2 = -0.373$. The first time scale $\tau_1 = 23 \text{ fs}$ describes the initial fast quantum delocalization process described above, while the second time scale $\tau_2 = 238 \text{ fs}$ the slower subsequent delocalization and the reaching of the equilibrium situation, $H(t = \infty) = \ln(3)$.

We now pass to systematically analyse the behaviour of the coherence of the evolution with respect to the strength of the interaction with the environment and its relevance for the energy transport process. As a first step we plot both $H(\tau = N\Delta t)$ and $C(\Delta t)$ for different values of $\gamma$, Fig. 3. The plots show that the coherence function exhibits the required behaviour: for small $\gamma = 0.1$, $C(\Delta t)$ oscillates with frequency $f_{+\rightarrow}/2$, following the Rabi oscillations of the dimer. The minima occur with $nf_{+\rightarrow}/4$, showing that the exciton is “partially” localized on site 1 or 2, and partially delocalized on site 3. As $\gamma$ grows, the system becomes unable to create coherence on large time scales; the decay of $C(\Delta t)$ is mirrored by a the reduction of the amplitude in the oscillations of $H(\tau = N\Delta t)$.

We now focus on the relevant time scales $\tau_d$ for the initial fast delocalization process highlighted by our previous analysis, and that are of the order of tens to hundreds of femtoseconds. We therefore introduce the following average measure of global coherence of the evolution

$$Q_{\tau_d}(\gamma) = \frac{1}{\tau_d} \int_0^{\tau_d} C(\Delta t) d\Delta t$$

$Q_{\tau_d}(\gamma)$ is the average of the coherence exhibited by the dynamics of the system at the time scales $\Delta t \in (0, \tau_d)$. In Fig. 4 it is shown $Q_{\tau_d}(\gamma)$ for the trimer (15) in site basis for different values of $\gamma$. 

Figure 2: For the trimer (15): a) Delocalization $H(t)$ and b) $p_3(t)$ population of site 3 as a function of time for different values of $\gamma = 0.1, 1, 16, 100$.
\[ \tau_d. \] We first focus on the behaviour of \( Q_{\tau_d}(\gamma) \) for a wide range of values of dephasing \( \gamma \in (0, 1) \); in this range, for small time scales \( \tau_d = 20 \) to \( 200 \) fs the average global coherence \( Q_{\tau_d}(\gamma) \) is approximately constant and equals the value attained in the full quantum regime i.e., \( Q_{\tau_d}(\gamma) \approx Q_{\tau_d}(\gamma = 0.1) \). For larger time scales \( (\tau_d \approx 1 \) ps) it rapidly decreases with \( \gamma \). This analysis shows that the behaviour of \( Q_{\tau_d}(\gamma) \) matches the expectations: the higher \( \gamma \) the smaller the time scales over which decoherence takes place, the lower the global coherence of the dynamics. Along with \( C(\Delta t) \) the functional \( Q_{\tau_d}(\gamma) \) is therefore in general a good candidate for the evaluation of the global coherence of open quantum systems evolution. As for the transport dynamics, we focus on the timescale identified with the analysis of \( \mathcal{H}(t) \) for optimal dephasing; for \( \tau_d = \tau_1 = 20 \) ps and \( \tau_d = 40 \) ps we see that the systems indeed retains most of the average coherence of the purely quantum regime up to the optimal values of decoherence \( (\gamma = 16 \) ps\(^{-1} \) in the figure), while it loses it afterward; this is a clear indication that this phenomenon is at the basis of the the fast intial delocalization process. Over longer time scales, the relevance of coherence is highly suppressed.

We now deepen our analysis about the relevance of the coherence of the evolution for the energy tranfer efficiency. To this aim we focus on the basic feature that distinguishes the classical and the quantum regime: interference. In particular we focus on the subblock \( D_3 \) of the decoherence matrix \( D \) pertaining to the third chromophore which describes the set of histories in site basis ending at site 3. Due to interference the probability of occupation of the site 3 at time \( \tau = N\Delta t \) can be written in terms of the the histories ending at site 3 \( p_3(\tau) = w_3(\tau) + \mathcal{I}_3(\tau) \), see (4).

In Fig. 5 we show \( \mathcal{I}_3(\tau) \) for different values of dephasing. One has different regimes: for \( \gamma \gg 1, \) the set of histories in site basis is fully decohered; \( \mathcal{I}_3(\tau) \approx 0, \) the histories do not interfere with
Figure 4: Average coherence of the evolution $Q_{\tau_d}(\gamma)$ for the trimer (15) for different values of $\tau_d$.

Figure 5: Left: interference $I_3(\tau)$ of histories ending in site 3 for the trimer (15) as a function of $\tau = N\Delta t$ for different values of $\gamma = 0.1, 1, 10, 100$; Right: $I_3(\tau)$ for different intermediate values of $\gamma$.

each other and $p_3(\tau) \approx w_3(\tau)$ i.e., the probability is simply the sum of diagonal elements of $D_3$. In the mainly quantum regime $\gamma \leq 1 \text{ ps}^{-1}$, $p_3(\tau) \neq w_3(\tau)$: after the initial positive peak the histories interfere with each other, globally the interference is mostly negative and therefore $p_3(\tau) \leq w_3(\tau)$.

For intermediate values of decoherence $\gamma^{-1} \approx 10 \text{ ps}$ the interference has a positive peak and then reduces to zero. While the first initial firngersnap of positive interference that takes place in the first $\approx 80 \text{ fs}$ is common for all curves corresponding to small and intermediate values of $\gamma$, the main effect of the bath is displayed after this initial period of time: the decoherence gradually suppresses interference, both the positive and the negative one; however for intermediate values of $\gamma$ the effect is stronger as for the negative part of the interference patterns. The environment thus implements what can be called a quantum recoil avoiding effect: it prevents the part of the exciton that, thanks to constructive interference, has delocalized on site 3 to flow back to the other sites.
In order evaluate possible advantage provided by the initial speed up in the delocalization process and by the interference phenomena showed above one has to take into account another relevant time scale of the transport process: the trapping time. Indeed, if the system is to take advantage of the fast delocalization due to the coherent behaviour, the exit of the exciton should take place on time scales of the order of the delocalization process. The theoretical and experimental evidences show that this is the case: the trapping time $k_{trap}^{-1}$ for the FMO complex is estimated in the literature to be of the order of 0.2 ps i.e., the exit of the exciton starts soon after the fast delocalization due to quantum coherence has taken place. The role of the interference between paths, in particular those leading to site 3, can therefore be appreciated by numerically evaluating

\[ \langle I_{\beta}^i \rangle = \frac{1}{\tau_{trap}} \int_0^{\tau_{trap}} I_{\beta}^i(\tau) d\tau \]  

i.e., the average over the trapping time scale of $\tau_{trap} = 200 \text{ fs}$ of the total ($\beta = Total$), negative ($\beta = -$) and positive ($\beta = +$) average interference between the histories ending in site $i$, with $\langle I_{\beta}^{Total} \rangle = \langle I_{\beta}^+ \rangle + \langle I_{\beta}^- \rangle$. In particular, in Fig. 6 (Left) the different kinds of interference are plotted for histories terminating at site 3: on average, the negative interference highly reduces the total interference for small values of decoherence strength; when $\gamma \approx 10 \text{ ps}^{-1}$, $\langle I_{3}^- \rangle$ vanishes, the average total interference equals the positive one $\langle I_{3}^{Total} \rangle = \langle I_{3}^+ \rangle$ and it is maximal for values of $\gamma$ comparable to those that maximise $H(t)$ ($\approx 16 \text{ ps}^{-1}$). In Fig. 6 (Right), we compare the behaviour of $\langle I_{\beta}^{Total} \rangle$ for all sites; the results again suggest that decoherence acts on the interference provided by the quantum engine in order to favour the flow of the exciton towards the exit chromophore: the average positive interference between histories ending at sites 2 and 3 grows in modulus with $\gamma$ and attains a maximum for intermediate values of decoherence; while the average negative interference between histories ending at site decreases and attains a minimum for intermediate values of $\gamma$. The combined effect of decoherence and interference thus helps depopulating site 1 and populate site 2 and 3.

We can now tackle one of the most relevant aspects of our discussion: the net effect of the above described phenomena on the overall efficiency of the transport. The latter can be fully appreciated by evaluating the efficiency of the process (14) and by recognizing that, in the decoherent histories language, it can be expressed as:

\[ \eta(t) = 2k_{trap} \int_0^t p_3(\tau) d\tau = W_3(t) + I_3(t) \]
where $\tau = N\Delta t$ and $W_3(t) = 2k_{\text{trap}} \int_0^t w_3(\tau) d\tau$, $I_3(t) = 2k_{\text{trap}} \int_0^t I_3(\tau) d\tau$; this split allows one to appreciate the role of interference for the efficiency. In Fig. (7) $\eta$ is plotted for different values of dephasing. In agreement with what discussed above, we have three regimes: for very small values of $\gamma$ the overall efficiency is poor; this is due to the presence of high negative interference that in average prevents the exciton to migrate to the exit site. For large values of $\gamma$ the interference processes are completely washed out and the system cannot take advantage of the fast quantum delocalization. For intermediate (optimal) values of $\gamma$ only the negative interference has been washed out: $I_3(\tau)$ is positive, it acts on short time scales, and it provides on average an enhancement of the global efficiency.

These results, within the limits of the simple model of decoherence taken into account, undoubtedly show for the first time that the so called ENAQT phenomenon can well and properly be understood both qualitatively and quantitatively within the decoherence histories approach i.e., in terms of very the basic concepts of coherence and interference between histories. The often recalled “convergence” of time scales or “Goldilocks” effect ([12]) in biological quantum transport systems seems therefore to be well rooted in the processes discussed above: if decoherence is too small the system shows both positive and negative interference, (see Fig. 2) the delocalization has an oscillatory behaviour, and the exciton bounces back and forth along the network thus preventing its efficient extraction. If instead decoherence is very high one has that the complete washing out of intereference and coherence implies the delocalization process to be very slow, no matter how fast the trapping mechanism tries to suck the exciton out of the system. In order to take advantage of the effects of quantum coherent dynamics: $i$) the bath must act on the typical time scales of quantum evolution in order to implement the quantum recoil avoiding process; $ii$) the extraction of the exciton from the complex, characterized by $k_{\text{trap}}$, must then start soon after the initial fast delocalization has taken place; should the extraction take place on longer time scales, the benefits of the fast initial delocalization would be spoiled since for waiting long enough, the system eventually would reach with the equilibrium a decent delocalization even for moderately high valued of $\gamma$; in this case the trasfer would be obviously much slower.

V. FMO

The above arguments can be easily applied to the whole FMO complex. As shown in Fig. 8 and 9 the main features of the behaviour of $C$, $H$, $Q$, $I_3$ and $\eta$ are maintained although obvious
VI. CONCLUSIONS

The focus of this paper is twofold. On one hand we introduce a novel theoretical framework to assess the (global) coherence properties of quantum (Markovian) evolution based on the well
known decoherent histories approach. In this context the main tools are based on the decoherence functional $\mathcal{D}$ and the interference between different histories. In particular we introduce the coherence functional $C(P,N,\Delta t)$ that can be interpreted as a measure of the global coherence exhibited by the dynamics in the basis $P$ over the time scale $\Delta t$. Based on $\mathcal{D}$ and $C(P,N,\Delta t)$ one can introduce: 

(a) a measure $Q_{\tau}(\gamma)$ able to characterize the average coherence exhibited by the dynamics of the system over the time scales $\Delta t \in (0, \tau)$ for fixed value of decoherence $\gamma$; 

(b) the measure of the average interference $\langle \mathcal{I}_i \rangle$ occurring between the histories ending at a given "site" $i$.

On the other hand we use these novel measures to assess the role of coherence in energy transport processes taking place in biological complexes, in particular the basic trimeric subunit of FMO. In this context we first thoroughly assess the consistency of the behaviour of $C(P,N,\Delta t)$ at the various regimes. We then study the intricate connections between the efficiency of the transport process and the coherence properties of the dynamics. In particular we show that the delocalization of the exciton over the chromophoric subunit is strongly affected by the amount
of (average) coherence allowed by the interaction with the bath in the first tens to hundreds of femtoseconds. If the system-bath interaction is too strong, coherence is suppressed alongside the interference between different histories, in particular those ending at the site where the excitation leaves the complex. If the interaction is too weak the system exhibits high values of coherence even on long time scales, but it also exhibits negative interference between pathways ending at the exit site, a manifestation of the fact that the exciton bounces back and forth over the network thus preventing its efficient extraction. In the intermediate regime i.e., when the different time scales of the system (quantum oscillations, decoherence and trapping rate) converge, the system shows high values of coherence on those time scales. The action of the bath has a quantum recoil avoiding effect on the dynamics of the excitation: the benefits of the fast initial quantum delocalization of the exciton over the network are preserved and sustained in time by the dynamics; in terms of pathways leading to the exit site, the action is to selectively kill the negative interference between pathways, while retaining the initial positive one. These effects can be explicitly connected to the overall efficiency of the environmentally assisted quantum transport: the gain in efficiency for intermediate (optimal) values of decoherence can thus be traced back to the basic concepts of coherence and interference between pathways as expressed in the decoherent histories language. These results are obtained within a simple (Haken-Strobl) Markovian model of decoherence, however we expect them to hold even in non-Markovian regimes where the coherence (interference) properties most likely are enhanced on the typical very short time of interest.

The tools introduced in this paper allow to thoroughly assess the coherence properties of quantum evolutions and therefore have very wide application, since they can be applied to generic quantum systems, the only limits being the restriction to Markovian dynamics and the computational efforts required for large systems. However, the extension to non-Markovian realms is indeed possible [30], and the use of parallel computing may allow the treatment of reasonably large systems.

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