The quantum Goldilocks effect: on the convergence of timescales in quantum transport

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Abstract: Excitonic transport in photosynthesis exhibits a wide range of time scales. Absorption and initial relaxation takes place over tens of femtoseconds. Excitonic lifetimes are on the order of a nanosecond. Hopping rates, energy differences between chromophores, reorganization energies, and decoherence rates correspond to time scales on the order of picoseconds. The functional nature of the divergence of time scales is easily understood: strong coupling to the electromagnetic field over a broad band of frequencies yields rapid absorption, while long excitonic lifetimes increase the amount of energy that makes its way to the reaction center to be converted to chemical energy. The convergence of the remaining time scales to the centerpoint of the overall temporal range is harder to understand. In this paper we argue that the convergence of timescales in photosynthesis can be understood as an example of the ‘quantum Goldilocks effect’: natural selection tends to drive quantum systems to the degree of quantum coherence that is ‘just right’ for attaining maximum efficiency. We provide a general theory of optimal and robust, efficient transport in quantum systems, and show that it is governed by a single parameter.

Keywords: Photosynthesis, quantum transport, decoherence.
Photosynthetic complexes are, by definition, complex [1]. They contain many light harvesting sub-complexes, each of which in turn contains multiple chromophores for storing and transporting excitons. Associated with the hierarchical arrangement of photosynthetic complexes is a diverse spread of time scales. The energy of the photons to be absorbed, and of the excitons created in the complex, corresponds to time scales of femtoseconds. The relaxation of the excitons to their ground states within a chromophore takes place over tens of femtoseconds. As noted above, a large number of processes in photosynthetic complexes take place over a fraction of a picosecond to several picoseconds, including hopping between neighboring chromophoric complexes, reorganization and relaxation in the bath of phonons, and decoherence. Similarly, energy differences between excitonic states of chromophores in different molecular environments typically correspond to picosecond time scales. The overall transfer time from absorption in the antenna to capture in the reaction center is tens of picoseconds. The entire process is limited by the excitonic lifetime, which is on the order of a nanosecond.

The time scales involved in photosynthetic processes span six orders of magnitude, from femtoseconds to nanoseconds, with a convergence of the time scales for many processes in the center of this range. Note that the these convergent processes are exactly those where the interplay between quantum coherence and decoherence in multi-body interactions can play an important role. Recent experiments, followed by detailed theoretical analyses, show that this interplay is crucial to excitonic transport in photosynthesis [2-10]. The purpose of this paper is to explain both the divergence of time scales in photosynthesis, and the convergence of the time scales for the particularly quantum processes at the picosecond range.

The functional purpose of divergent time scales is easy to understand. Efficient absorption of light over a broad band of frequencies requires both strong coupling of light to excitons, i.e., large induced dipole moments, and broad bandwidths for absorption, i.e., rapid relaxation. The stronger the coupling, and the broader the absorptive bandwidth, the more energy available to the bacterium or plant performing photosynthesis. Accordingly, we should not be surprised that over time, natural selection leads to fast time scales associated with absorption of light and creation of excitons. Similarly, the large separation between the time scale for creation of excitons and the time scale for their eventual decay should come as no surprise: the longer the excitonic lifetime, the more likely it is to make it from the photosynthetic antenna to the reaction center before decaying.
The functional purpose of the convergence of time scales is harder to understand, for the simple reason that convergence of time scales makes quantum systems hard to model. Our ability to make simplified, perturbative models of complex quantum systems hinges crucially on the separation of time and energy scales, so that quantum effects with divergent time scales can be regarded as perturbations on each other. From the perspective of a scientist trying to analyze excitonic transport in photocomplexes, the convergence of time scales seems almost to be an effort on the part of nature to frustrate our understanding. Nature is modest and keeps her secrets well. Independent of nature’s intrinsic modesty, however, the convergence of time scales can play a functional role in enhancing excitonic transport – or any other form of transport. When the time scales for two processes converge – e.g., coherent tunneling time and decoherence time – then the two processes affect each other strongly. The convergence of time scales can then either assist energy transport, or interfere with it. In naturally occurring systems that have undergone a long process of dynamic refinement via natural selection, the convergent processes typically help each other out.

Recently, we developed a non-perturbative, non-Markovian master equation technique for simulating the behavior of complex quantum systems over a wide variety of time and energy scales [9]. We applied this technique to the Fenna-Matthews-Olson complex (FMO), a seven-chromophore energy transport complex in green sulphur bacteria [10]. In that work, we found that the convergence of timescales in FMO is tuned to give high transport efficiency (virtually 100%) that is robust over several decades of variation in the underlying parameters of the system. A similar study has also shown the optimality of energy transfer efficiency in the FMO complex [11]. Moreover, the efficiency of transport was shown in [9-10] to be a function of a single underlying parameter that is linear in the various timescales themselves. The purpose of this paper is give a heuristic but quantitative derivation for how convergence of timescales yields optimal and robust transport.

The paper is organized as follows. First, we review the classical Goldilocks principle for complex, designed systems, explaining why it is important to attain just the right level of complexity [12-14]. Second, we review the theory of environmentally assisted quantum transport (ENAQT), which gives the underlying theoretical mechanism for robust and efficient excitonic transport [5-8]. Finally, we give a heuristic analysis of how different timescales enter into the transport process to derive the quantum Goldilocks principle: efficiency is optimized at just the right level of quantum coherence. We confirm the existence
of a single parameter that governs transport in complex, partially ordered quantum systems [9-10], and show why this parameter takes its particular form as a ratio of products of the different time and energy scales in the system. Because of the simple functional form of the parameter governing the efficiency of transport, optimal transport rates – approaching 100% in biological systems – can be readily attained by natural selection. At any point of evolution, there are many paths towards the global optimum of transport efficiency, and there are no local optima in which to be trapped along the way.

The Goldilocks principle for complex, designed systems

The story of Goldilocks and the three bears was published by the English poet Robert Southey in 1837, although it is presumably a variation on a much older folktale. In the version known today, a small girl with blonde hair, Goldilocks, is lost in a forest. She finds a house whose inhabitants have just left it. The house contains three of everything – there are three chairs, three bowls of porridge sitting on a table, three beds, etc. One of the chairs is too big for Goldilocks, one too small, and one just the right size. So she sits on the one that is just right. One of the bowls of porridge is too hot, one too cold, and one just the right temperature. So she eats the one that is just right. One of the beds is too hard, one too soft, and one just the right degree of firmness. So she lies down on the one that is just right and falls asleep. At this point the three bears arrive home and . . . – the ending ranges from gruesome to happy depending on the version.

The Goldilocks principle states that, given a choice between alternatives, one should choose the one that is ‘just right’ for the purpose at hand. Applied to complex systems that are adapted to a particular set of functions, the Goldilocks principle states that there is a level of complexity that is just right [12]. If the adapted system is too simple, then it will fail to attain its various functions. If it is too complex, then it will be expensive and lack robustness. When the complex system in question is one designed by human beings – a car, for example – then the Goldilocks principle is embodied by the widely applied theory of axiomatic design [13-14]. In this theory, one looks at the design matrix that relates input design parameters to output functional parameters. If one wishes to attain a target set of functional parameters in a $D$-dimensional space, then one needs to be able to vary at least $D$ design parameters independently to attain that target. More than $D$ design parameters yields redundancy and unwanted complexity.

In the case of biological systems that have undergone many generations of functional refinement via natural selection, we expect the Goldilocks principle also to hold. Biological
systems evolve to the level of complexity required to attain their necessary functions within their ecological niche. Having attained the requisite level of complexity, they only add new features or increased complexity if by doing so they can obtain a competitive advantage within that niche.

In this paper, we argue that energy transport in photosynthesis – a process that is, at bottom, quantum mechanical – has attained the level of quantum coherence and complexity that is just right for attaining high efficiency (in some cases, almost 100%) of transport of excitons from the antenna to the reaction center. In particular, the interplay between coherent dynamics and environmental interaction attains just the right level of quantum coherence to insure high transport efficiency. We show that the mechanism for this quantum Goldilocks effect arises from the phenomenon of environmentally assisted quantum transport (ENAQT), a mechanism that intrinsically gives rise to efficient and robust transport over a range of the various quantum timescales of the photosynthetic complexes [5-8]. Using a heuristic but quantitative argument, we show that the transport efficiency is governed by a single parameter that is a linear function of these timescales and the corresponding energy scales. Because of the linear dependence of the efficiency parameter on the different timescales, natural selection can arrive at optimal values for this parameter by adjusting timescales in the proper direction until optimality is attained – that is, there are no sub-optimal local maxima to the efficiency. Elsewhere, we show that this heuristic argument is supported by detailed simulations of photosynthetic complexes [9-10]

Optimal timescales for quantum transport

The fundamental mechanism that we propose governs the efficiency of transport is environmentally assisted quantum transport (ENAQT) [5-8]. ENAQT operates by an interplay between coherence, decoherence, and disorder in quantum systems. Up to now, our work on environmentally assisted quantum transport has been based on detailed simulations of specific systems such as FMO. Here we provide a simple mechanism for understanding quantitatively the interplay between coherence, decoherence, and disorder.

Consider a quantum walker such as an exciton, moving through an array of sites. The array can be in one, two, or more dimensions; it can possess a fractal dimension, or exhibit different dimensions at different length scales. It can be large or small. The quantum walk can take place by local or by non-local interactions, as in the dipolar interaction, as long as nearest neighbor interactions are the strongest ones.
Let $J$ be the average strength of coupling between neighboring sites, and assume that the coupling between distant sites falls of relatively rapidly (for example as in dipolar coupling). Let $\ell$ be the transient localization length of the system: $\ell$ is the typical length of a path over which the walker can propagate coherently before being localized by destructive interference. In a system that exhibits Anderson localization [15], the transient localization length is equal to the normal localization length. However, as discussed below, even systems that do not exhibit strict Anderson localization still exhibit transient localization. The transient localization length can be different in different parts of the system. For the analysis here, assume that $\ell > 1$, so that the walker can propagate at least one full step before being localized. The case of strong transient localization, $\ell < 1$, will be discussed below. The amount of time it takes to propagate along the localization length $\ell$ is $\tau \approx \ell / 2J$, (for $J$ measured in Hertz).

In the absence of environmental interactions, the system propagates coherently over the localization time $\tau$ a distance equal to the localization length $\ell$, and then becomes stuck due to destructive interference. Decoherence can then ‘free up’ the system and allow it to propagate further. Call the environmental decoherence rate $d$. The ENAQT mechanism suggests that there should be an optimal rate of decoherence.

We estimate the optimal rate of decoherence by the following simple argument. If the decoherence time is longer than the localization time, $d < 1/\tau$, then the walker propagates a length $\ell$, becomes stuck due to localization, and waits around for a time $1/d$ to become unstuck. At this point it can propagate coherently for the localization length again, and the process continues. Such a process corresponds to a classical random walk with step size $\ell$ and step time $1/d$, leading to diffusion over time where $r(t) \approx \ell \sqrt{t/d}$. In this regime, increasing the decoherence rate increases the propagation rate.

Conversely, if the decoherence time is shorter than the localization time, $d > \tau$, then the walker propagates coherently for a number of steps $2J/d < \ell$ before getting decohered. By the same argument as before, it then takes a classical random walk with step size $2J/d$ and step time $1/d$, yielding diffusion over time $r(t) \approx (2J/d) \sqrt{t/d} = (2J) \sqrt{t/\ell}$. In this regime, decreasing the decoherence rate increases the propagation rate.

The optimal rate of decoherence is seen to occur for $d \approx 1/\tau$. That is, the decoherence time is equal to the localization time – no more, no less. Setting the decoherence time equal to the localization time gives the interplay between coherence and decoherence that is ‘just right.’ When $d \approx 1/\Delta t = 2J/\ell$, the walker takes a classical random walk with step
size ℓ and step time 1/d = ℓ/2J = Δt, yielding diffusion over time as

\[ r_{\text{opt}}(t) \approx \ell \sqrt{td} = \ell \sqrt{2tJ/\ell} = \sqrt{2tJ\ell}. \]  (1)

Equation (1) gives the optimal rate of propagation when the quantum Goldilocks principle is satisfied.

When the coupling between neighboring sites is less than the energy splitting between them, i.e., \( J < \Delta \omega \), then coherent transport is strongly suppressed: the walker has a relatively small amplitude of transiting to a neighboring site. A simple two-state model then shows that the maximum probability of transition goes as \( J^2/\Omega^2 \), where \( \Omega^2 = J^2 + \Delta \omega^2 \), and occurs at time \( \Delta t = 1/2\Omega \). As before, the optimal decoherence rate goes as \( d \approx 1/\Delta t \). When \( J \ll \Delta \omega \), the optimal decoherence rate simply matches the average energy disorder \( \Delta \omega \) of the system. At the optimal rate, takes a step with probability \( J^2/\Omega^2 \) at time intervals, \( \Delta t = 1/2\Omega \), yielding random walk that spreads as \( J \sqrt{2t/\Omega} \).

Note the environmentally assisted quantum transport is an intrinsically robust mechanism. The optimum transport occurs when the parameter \( \Lambda \equiv d\ell/2J \approx 1 \), but optimality extends over a considerable range of values of \( \Lambda \). Our FMO simulations show high efficiency of transport for \( 0.2 < \Lambda < 5 \).

### Transient localization

As noted above, for our purposes it is not necessary that the system exhibit strict Anderson localization [15]. Essentially any disordered quantum system exhibits transient localization over the time scale required for destructive interference to build up. Transient localization occurs even when systems have long-range interactions, or exist in dimensions where strict Anderson localization does not take place. The transient localization length can be estimated as follows. Localization arises from disorder in energy. Disorder in coupling constants and in the topology of the graph also play a role. For the moment consider the effect of energy disorder, \( \hbar \delta \omega \). The transient localization length is a function of \( J/\Delta \omega \). In particular, over the time scale \( 1/2J \) required for the walker to propagate from one site to the next, it acquires a random phase \( \pm \pi \Delta \omega / J \). After \( n \) steps, the walker acquires a phase \( \pm \sqrt{n\pi} \Delta \omega / J \). Transient localization occurs when paths of propagation become sufficiently long to acquire a random relative phase. That is, transient localization occurs when \( \sqrt{\ell \pi} \Delta \omega / J \approx \pi \), so that the transient localization length goes as \( \ell \approx (J/\Delta \omega)^2 \) and the localization time goes as \( \tau \approx J/2\Delta^2 \). The optimal decoherence rate is \( d = 1/\tau = 2\Delta \omega^2 / J \), and the optimal transport rate goes as \( \sqrt{2tJ\ell} = (J/\Delta \omega)\sqrt{2tJ} \). When disorder in coupling
constants and in energy are included, the transient localization length decreases and the estimate $\ell \approx (J/\Delta \omega)^2$ is now an approximate upper bound on the localization length.

Even when energies and couplings are identical, transient localization can also occur due to disorder in the network of sites through which the walker is propagating, or due to quantum chaos [16-17]. As an example of transient localization, consider dipolar interactions such as those that occur in photosynthesis. Dipolar systems have long range interactions and will not be localized in the long run. Initially, a disordered quantum system exhibits coherent propagation from the dominant, short range part of the dipolar interaction. Destructive interference effectively freezes this propagation at a characteristic time scale equal to the time needed for destructive interference to build up. Over much longer times, the long range part of the interaction allows the walker to ‘leak out’ of its transiently localized state. For excitons propagating through photocomplexes, however, the time scale for the destruction of transient localization by long range interactions is typically longer than the exciton lifetime. In the long run, transient localization goes away. But in the long run, the excitons are all dead.

Transient localization also plays a role in systems that are too small to exhibit strict Anderson localization. For small systems, the transient localization length can be determined by identifying the number of sites that participate in energy eigenstates of the system. The localization length can differ from place to place within the system. The average energy splitting difference between the $\ell$ excitonic states in a band delocalized over $\ell$ sites is $\Delta E \approx 2\pi \hbar J/\ell$. Accordingly, our quantum Goldilocks criterion $d\ell/2J \approx 1$ that the decoherence rate match the coherent propagation time is equivalent to asking that the $\pi \hbar d$ be equal to the average energy splitting $\Delta E$ between exitonic states in a band delocalized over $\ell$ sites.

Phrased in terms of localized excitonic states, the criterion $d\ell/2J \approx 1$ has simple explanation: it states that transport is optimized when the local decoherence rate is approximately equal to the local splitting in frequency between excitonic states in a band. That is, the optimal rate of decoherence is to ‘fuzz out’ the local energy levels until they begin to overlap with each other, and the noise has sufficient spectral width to induce transitions between excitonic states. Note that this explanation does not rely on relaxation. Relaxation can also play an important role in transport, particularly when the target state is at a lower energy than the input states, as in FMO. However, as shown in [5-10], the interplay between coherence and pure decoherence is surprisingly effective in arranging
robust and efficient energy transport.

As noted above, localization lengths, energy splittings, and decoherence rates can vary throughout a system. When there is such variation, optimal transport is attained by matching

\[ d \approx 2J/\ell \approx \Delta E/\pi \hbar \]

locally throughout the system.

**Convergence of time scales**

The theory of open quantum systems implies that the decoherence rate at high temperatures – which include the temperatures physiologically relevant for photosynthesis –

\[ d = \alpha \lambda kT/\hbar^2 \gamma, \]

where \( \lambda \) is the reorganization energy which measures the strength of the interaction between system and environment, \( T \) is the temperature, \( \gamma \) is the inverse bath correlation time, and the proportionality constant \( \alpha \) is \( O(1) \) and depends upon the spectral density of the environment, degree of non-Markovianity, etc. For example, an uncorrelated local ohmic spectral density with frequency cutoff yields \( \alpha = 2\pi \) [6]. This dependence of decoherence rate on fundamental parameters follows in a straightforward way from second order perturbation theory in the Markovian limit [6, 18-19]. However, as shown in [9-10, 19], it can also capture the decoherence rate in non-perturbative, non-Markovian scenarios, although with a different proportionality constant.

The bath correlation length is also important: if the fluctuations that induce decoherence in neighboring sites are positively correlated, then the effective relative decoherence rate is reduced. Similarly, when the correlations are negatively correlated, the effective relative decoherence rate is increased. Let \( c \) be the normalized correlation coefficient of the fluctuations, so that \( c = 1 \) corresponds to perfect correlation between neighboring sites, \( c = -1 \) corresponds to perfect anti-correlation, and \( c = 0 \) corresponds to no correlation. Taking into account the spatial correlations between sites yields a relative decoherence rate between neighboring sites,

\[ d = \alpha (1 - c) \lambda kT/\pi \gamma \hbar. \]

Transport is optimized when

\[ d \approx 2J/\ell \approx \Delta E/\pi \hbar, \]

where as above, \( \Delta E \) is the average energy splitting of excitonic states in a band delocalized over \( \ell \) sites. The optimum occurs when the single parameter

\[ \Lambda = d\ell/2J = \alpha (1 - c) \lambda kT/\hbar \gamma \Delta E \approx 1. \] (2)

As noted, the analysis of optimality in quantum transport applies to a wide variety of systems. The transport could take place over a quasi-one-dimensional chain, as in a single
LH1 or LH2 ring is quasi-one-dimensional. The couplings, disorder/energy splittings, and decoherence rates need not be distributed uniformly throughout the complex in general (with the exception of symmetric complexes such as LH1 and LH2). The above heuristic analysis should continue to hold, however, as long as one looks at transport over individual energy pathways within a complex. For example, in LHCII, the primary light-harvesting complex of green plants, the various energy pathways within an LHCII monomer pass through sequences of relatively localized and relatively delocalized states, corresponding to more weakly coupled chromophores and to groups of more strongly coupled chromophores, respectively. The analysis above can then be applied to analyze the efficiency of transport along the energy pathway step by step, as the exciton propagates incoherently between weakly coupled chromophores, and then semi-coherently along bands of delocalized states. For each step, we expect transport to be maximized for the decoherence rate approximately equal to the disorder/energy difference associated with that step.

The complex and partially disordered quantum nature of photocomplexes implies that a numerically accurate theoretical picture of transport requires detailed simulations with the appropriate open quantum system techniques, e.g., the non-perturbative, non-Markovian master equation techniques mentioned above. Applied to FMO, such simulations [9-10] are consistent with the heuristic arguments given here.

Transport and the quantum Goldilocks effect

As noted in [5-8] environmentally assisted quantum transport intrinsically gives rise to high efficiencies over a relatively wide range of parameters. As long as the amount of time it takes the exciton to diffuse throughout the photocomplex is significantly less than the exciton lifetime, then the efficiency will be close to one. From equations (1-3), we see that transport is optimized by matching the decoherence time with the localization time, which is equivalent to making the energy splitting within a localized band of excitons comparable to the spreading of energies due to decoherence. X-ray crystallography of photocomplexes, together with quantum studies of excitonic states in chromophores, indicates that chromophores are packed pretty much as closely as possible within photocomplexes – if they were packed more closely, excitonic wave-function overlaps between chromophores would lead to quenching and energy loss. That is, naturally occurring photosystems have evolved to a structure that effectively maximizes the couplings between chromophores. Detailed laser spectroscopy of photocomplexes suggests the disorder/energy splitting in such complexes is indeed comparable to the decoherence rate [2-4].
The degree of coherent propagation differs from photocomplex to photocomplex. The coherent propagation length is largest in strongly coupled chromophore arrays with a high degree of symmetry, such as $LH1$ and $LH2$ rings, or the green sulphur bacteria chlorosome. Larger couplings and regular arrangements of chromophores lead to excitonic states that are delocalized over a larger number of sites, and the possibility for coherent propagation of excitons between those sites. By contrast, the coherent propagation length is smaller in more weakly coupled and more diversely structured photocomplexes such as $FMO$ or $LHCII$, where energy funnels also play a role. Weaker coupling and less regular structure lead to more localized states and to shorter coherent propagation lengths. In systems with significant energy differences between input excitons and output states, relaxation can significantly affect efficiency of transport, as well as decoherence. Interestingly, however, our detailed simulations of FMO [9-10] show that even when there are significant energy difference, the interplay between coherence and decoherence can largely determine the efficiency of transport.

As shown above, the efficiency of transport is governed by the parameter $\Lambda = d\ell/2J$ for systems with a localization length $\ell$ considerably larger than one, and by $\Lambda = d/2\Omega$ for highly localized systems, where $\Omega^2 = J^2 + \Delta\omega^2$. FMO is a relatively highly localized system, with typical energy splittings between chromophores larger than their couplings. Engel et al. have measured the decoherence rate in FMO for quantum beating at physiological temperatures [4], and have found values $d = 270 \pm 100 \text{cm}^{-1}$ for a transition with frequency $\Omega = 173 \pm 18 \text{cm}^{-1}$, yielding $\Lambda \approx 0.8 \pm 0.3$, consistent with the value 1.

We would like to estimate $\Lambda$ for systems where the transient localization length $\ell$ is greater than one, for which $\Lambda = \tau d = \ell d/2J$. In the 850 nanometer ring of LH2, for example, excitons are delocalized over multiple sites in the ring. Strümpfer and Schulten [19] calculate the time it takes an exciton to spread from a single site to half the ring (nine sites) as $\approx 150$ femtoseconds, suggesting a localization time of $\approx 100$ femtoseconds if the localization length is somewhat less than half the ring. That is, the strong coupling between chromophores in LH2 make for longer transient localization lengths and shorter localization times than in FMO. We can now use the generic form of the decoherence rate at physiological temperatures $T d = \alpha(1 - c)\lambda kT/\hbar^2 \gamma$ to estimate $\Lambda$ in LH2. Strümpfer and Schulten [20] report the following values for FMO: $\lambda = 35 \text{cm}^{-1}$, $\gamma = 50 \text{cm}^{-1}$. For the 850 nm ring of LH2, they report $\lambda = 200 \text{cm}^{-1}$, $\gamma = 83 \text{cm}^{-1}$, suggesting a decoherence rate several times faster for LH2 than for FMO (assuming that the proportionality constant $\alpha$
takes on similar values for the two distinct systems). But as just noted, they also estimate the coherent propagation time to be several times shorter for LH2 than for FMO, once again suggesting $\Lambda \approx 1$.

The green sulphur bacteria chlorosome consists of regular cylindrical arrays of tightly coupled chromophores, which might exhibit coherent propagation of excitons over significant scales. Simulations of the interplay of coherence and decoherence in cylindrical and spiral arrays of chromophores in the presence of disorder show clear evidence for the destruction of localization via the addition of decoherence [21], with optimal transport for decoherence rates approximately equal to the inverse localization time.

The reorganization energy, correlation time of environment, and disorder/energy splitting, are all parameters that have the potential to be tuned by natural selection. Decoherence rates differ throughout the photocomplex: our model predicts that these rates – if optimized by natural selection – should correspond to to the exciton splitting in localized bands. The simple form of $\Lambda$ as the ratio of fundamental quantum parameters shows that optimum transport can be attained simply be evolving each of the parameters in the right direction until $\Lambda = 1$ is reached – there are no false maxima at relatively low efficiency.

Discussion

This paper discussed the divergence and convergence of time and energy scales in quantum transport processes. The convergence of time scales can be thought of as an example of the quantum Goldilocks effect, which states that there is a ‘just right’ level of quantum complexity and coherence for functional complex quantum systems such as photosynthetic complexes. When the time scales for different quantum processes converge, these processes can help each other out to give more efficient transport.

We then analyzed a potential mechanism of attaining robust, efficient quantum transport. Environmentally assisted quantum transport (ENAQT) uses the interplay between coherence and decoherence to attain efficiency and robustness [5-10]. We gave a heuristic but quantitative argument that showed that the efficiency of transport can be increased (a) by increasing the coupling between sites, (b) by minimizing disorder and energy splitting, and (c) by setting the decoherence rate equal to the disorder/energy splitting. This heuristic argument complements the detailed simulations presented in [9-10,18]. We showed that transport efficiency at high temperatures is a function of the single parameter $\Lambda = d\ell/2J \approx \alpha(1 - c)\pi\lambda kT/h\gamma \Delta E$, where $d$ is the decoherence rate, $\ell$ is the transient localization length, $J$ is the local coupling, $c$ is the correlation coefficient for noise between
neighboring states, $\lambda$ is the reorganization energy, $T$ is the temperature, $\gamma$ is the inverse correlation time of the environment, and $\Delta E$ is the energy splitting within a localized band of states, and $\alpha$ is a constant of order one. High efficiency is attained for $\Lambda \approx 1$. This simple set of rules for increasing quantum transport efficiency together with the simple form for the governing parameter $\Lambda$, provides a straightforward path for natural selection to implement the quantum Goldilocks effect – there is only one broad optimum for the ratios of values, and changing any one of the timescales in the system to make $\Lambda$ closer to one will typically increase efficiency. While this paper focused on excitonic transport in photosynthetic complexes, the heuristic, quantitative analysis given can be applied to any quantum transport process, in relatively complex quantum systems that exhibit a combination of order and disorder. The quantum Goldilocks effect can be used to maximize efficiency and minimize energy dissipation in any process in which a quantum system progresses through a sequence of quantum-mechanical states in order to accomplish some function. For example, conformational changes in proteins or in optically active molecules such as retinal can be accelerated by the proper balance of coherence and decoherence. The quantum Goldilocks effect is not confined to systems that have been optimized by natural selection: the principles for maximizing transport efficiency described here for evolved systems could also fruitfully be applied to the design of artificial energy harvesting systems.

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