

Efficient Energy Transport in Photosynthesis

Roles of Coherence and Entanglement

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Abstract

Recently it has been discovered—contrary to expectations of physicists as well as biologists—that the energy transport during photosynthesis, from the chlorophyll pigment that captures the photon to the reaction centre where glucose is synthesised from carbon dioxide and water, is highly coherent even at ambient temperature and in the cellular environment. This process and the key molecular ingredients that it depends on will be described. By looking at the process from the computer science view point, we can study what has been optimised and how. A spatial search algorithmic model based on robust features of wave dynamics will be presented.

G.S. Engel et al., Evidence for Wavelike Energy Transfer through Quantum Coherence in Photosynthetic Systems, *Nature* 446 (2007) 782-786.

E. Collini et al., Coherently Wired Light-harvesting in Photosynthetic Marine Algae at Ambient Temperatures, *Nature* 463 (2010) 644-647.



Photosynthesis

Light harvesting complexes of photosynthetic organisms direct the captured photon energy, from an antenna of pigment molecules to the reaction centre.

The energy is used to dissociate water (into H^+ and OH^-) and create charge separation across a membrane, which drives chemical processes for the synthesis of glucose.

The process has >95% energy utilisation efficiency.

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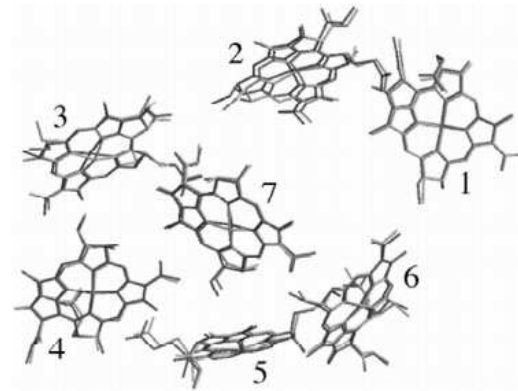
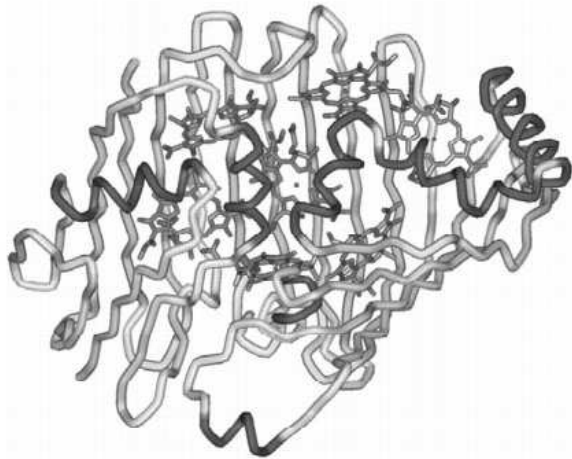
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Antenna arrangement of pigment molecules (in 3-dim):

- Increases harvesting area for expensive reaction centres.
- **Allows variations in light direction, intensity and frequency.**
- Permits accumulation of energy at the reaction centre.
- **Compensates for dead time after photon absorption.**
- The geometry is not that of a star/ring/regular graph.

The pigment molecules are coupled to neighbours, and the reaction centre is next to one of the pigment molecules.





The Fenna-Matthews-Olson antenna complex.

Left: With the protein scaffold in the ribbon representation.

Right: Only the pigment molecules without the scaffold.

The reaction centre is next to pigment 3.

Multiple energy transport pathways exist.

The major ones are: 6 – 5 – 7 – 4 – 3 and 1 – 2 – 7 – 3.



Energy Transport

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Fleming et al.: Purple bacteria, containing FMO protein with 7 bacteriochlorophyll pigment molecules, at 77K.

Scholes et al.: Marine cryptophyte algae, containing PC645 and PE545 proteins with 8 bilin molecules, at 294K.

Video of 2-dim spectroscopy: Coherence and beats



Excitons

Excitons are extended molecular (not atomic) states, often spanning two molecules over nanometre distances.

All exciton energies are not equal, but coherent energy transport (back and forth) still occurs. In the process, small decoherence/damping is clearly visible.



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The exciton energy has to accumulate without dissipation, and remain at the reaction centre for duration long enough (\sim few ps) for conversion to chemical form.

Can we formulate a realistic algorithm?



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Discrete Boolean logic is implemented using digital circuits.



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A practical implementation needs a trade-off between (i) minimisation of resources, and (ii) minimisation of errors.



Wave Algorithms

	Resources	Stability
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Wave systems with coupled vibrational (and rotational) modes, and small damping, can be made easily.

Efficient schemes to transfer/redistribute energy can have many practical applications—from mechanical systems to chemical, electrical and biological ones.

Living organisms are not systems in thermal equilibrium, and they perform efficient free energy processing to stay out of equilibrium (in order to survive, prosper and reproduce).



Coherence vs. Entanglement

A generic state in N -dimensional Hilbert space is

$$|\psi\rangle = \sum_{i=1}^N c_i |i\rangle.$$

Coherence: Relative phases of c_i are protected.
(off-diagonal density matrix elements)

Entanglement: The state cannot be factorised.
(specific to a choice of subsystems)

$$N = \begin{cases} N_1 \times N_2 & \text{Entanglement possible} \\ 1 + 1 + \dots + 1 & \text{Superposition without entanglement} \end{cases}$$



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Wave algorithms can be useful in situations where

- (i) quantum algorithms are fragile,
- (ii) oracles are expensive,
- (iii) spatial resources are cheap, and
- (iv) problem size (no. of required modes) is modest.



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Grover's algorithm: An unsorted database of N items can be optimally searched using $(\pi/4)\sqrt{N}$ binary questions. The algorithm can be implemented either using entangled qubits or using coupled oscillator modes.



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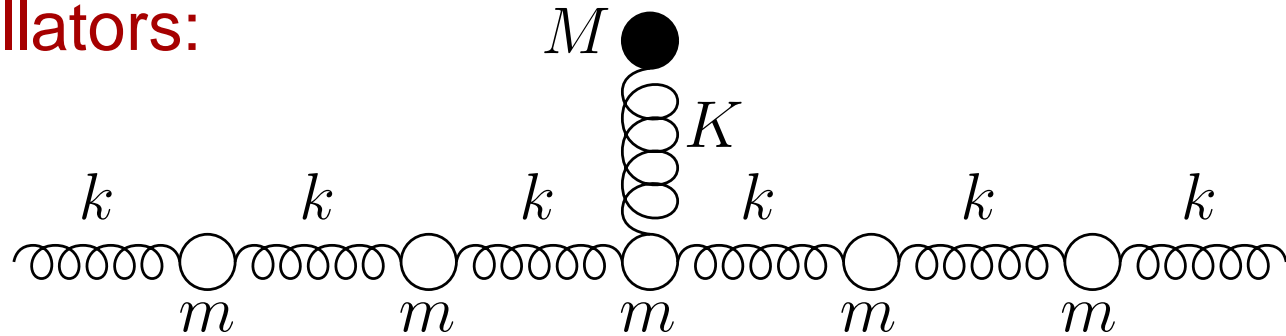
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With simultaneous constraints of unitarity (quantum theory) and bounded speed of movement (special relativity), the best algorithms are found in the formalism of relativistic quantum mechanics.



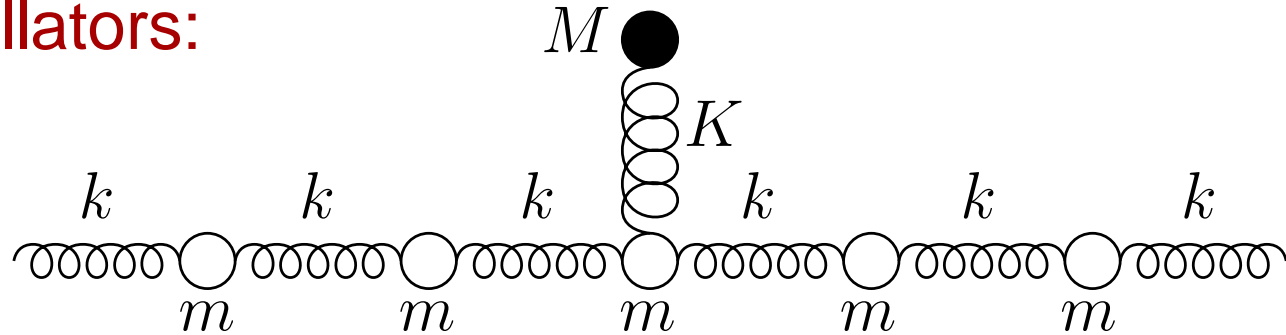
A Coupled Oscillator Model

Set of oscillators:

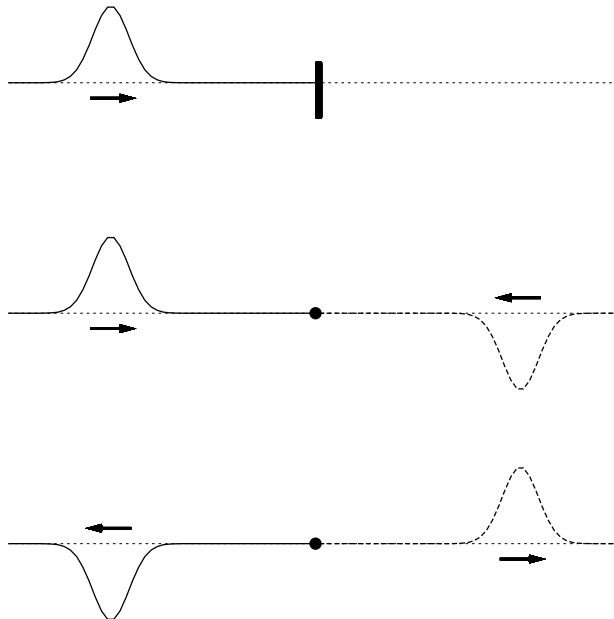


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Reflection oracle:



Ingredients

(1) The charge density ($\rho = \psi^* \psi$) does not carry the electronic wavefunction phase, which decoheres rapidly.

(Classical modes belong to the “decoherence free” subspace of the quantum modes.)

(2) But it carries the more robust vibrational phase.

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(4) Tulsi’s algorithm: Wave motion in a coupled oscillator system can be trapped at a specific location.

(Ancilla control/position dependent mass/self-loop at the oracle site/Fabry-Pérot cavity)

(5) Number of oscillators, their connectivity and coupling parameters can be optimised for best solutions.

(Interfering contributions have to be in phase for build-up at the oracle site.)



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These estimates are invalid for frequent interactions (what is supposed to escape irreversibly may return), as well as for adiabatic interactions (phase disturbances cancel restoring interference for cyclic evolutions).

Only environment modes with evolution time scales comparable to that for the system contribute significantly to decoherence of waves.

