A Wave Model for Efficient Energy Transport in Photosynthesis

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Quantum Physics of Living Matter

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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. By looking at the process from the computer science view-point, we can analyse what has been optimised and how. The hardware needs to be stable against environmental decoherence, and the software corresponds to the spatial search algorithm. Both of these can be realised in the framework of wave computation.

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The light harvesting antennae function by propagation of excitons through dipole-dipole interactions, and accumulation of energy at the reaction centre. As a concrete example, a coupled oscillator model implementing wave dynamics is presented. It executes the spatial search algorithm with nearest neighbour coupling and a reflection oracle. Its dynamics concentrates the energy of the system at the target location, analogous to the trapping mechanism of a resonating cavity. Geometry and connectivity of the coupled oscillators are the features to be optimised, while the resonance condition has to be met to make the process highly efficient. These algorithmic requirements can be tested against physical properties of the light harvesting antennae.

Keywords: Light harvesting antenna, Decoherence, Spatial search, Wave computation, Coherent state, Resonating cavity.

Photosynthesis

Light harvesting complexes of photosynthetic organisms capture photons, and direct the 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.

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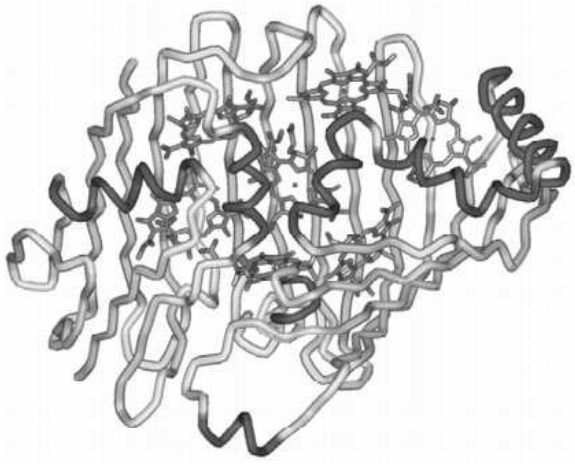
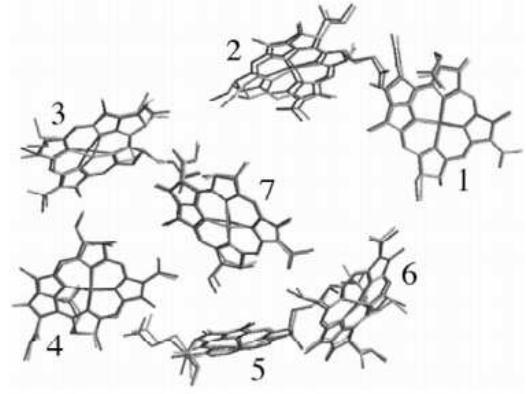
In the 3-dim antenna arrangement, the pigment molecules are coupled to their neighbours via a rigid protein scaffold.

Geometry and connectivity of the network are the key ingredients in the efficient energy transport process.

Fenna-Matthews-Olson Complex





Left: With the protein scaffold in the ribbon representation.
Right: Only the pigment molecules without the scaffold.

The geometry is not that of a regular graph. The reaction centre is next to pigment 3.

Major energy transport pathways are: $6-5-7-4-3$ and $1-2-7-3$.

The Antenna Structure

Visible light wavelength is much larger than the separation between pigment molecules. So several pigment molecules can capture a given incident photon.

Advantages of the antenna arrangement:

- Increases harvesting area for expensive reaction centres using cheap pigment molecules.
- Handles variations in light direction and frequency.
- Protects against high intensity by partial switch-off.
- Compensates for dead time after photon absorption.
- Allows multiple energy transport pathways.
- Permits accumulation of energy at the reaction centre.

(Energy of 4-5 photons is needed to dissociate water.)

Sophisticated telescopes also use an antenna of detectors for high sensitivity.

Energy Transport

Hopping distances are ~ 20Å. Transfer times are ~ 50fs.
Classical strategy of an energy funnel from the antenna of pigment molecules towards the reaction centre is expensive (requires maintenance of permanent energy gradients).
A non-dissipative transport needs an energy trap
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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.

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The polarisation cloud propagates through dipole-dipole interactions. Vibrational modes arise from tight covalent binding of the pigment molecules with the protein scaffold.

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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. (Sufficient build-up of polarisation ultimately dissociates water.)

Can we construct a computational model?

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

Coherence vs. Entanglement

A generic state in an $N-$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)

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All wave processes suffer decoherence and damping due to interaction with the environment. Generically, superposition is much more stable than entanglement, and decoherence is much more rapid than damping.

Wave Algorithms

Wave and quantum algorithms can cover the same Hilbert space. The two have the same time and oracle complexity, but different space requirements.

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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 equibilbrium, and they perform efficient free energy processing to stay out of equilibrium (in order to survive, prosper and reproduce).

Wave Computation

Wave algorithms can be useful in situations where
(i) the problem size (no. of required modes) is modest,
(ii) the spatial resources are cheap, and
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Algorithms can be implemented using coupled oscillator modes (in contrast to entangled qubits).
Number of oscillators, their connectivity and coupling parameters are the design parameters to be optimised.

Spatial Search

Search algorithms locate a target item in a database.

The items may be distributed over many distinct physical locations (as opposed to internal space labels).

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Geometry and connectivity are important features.

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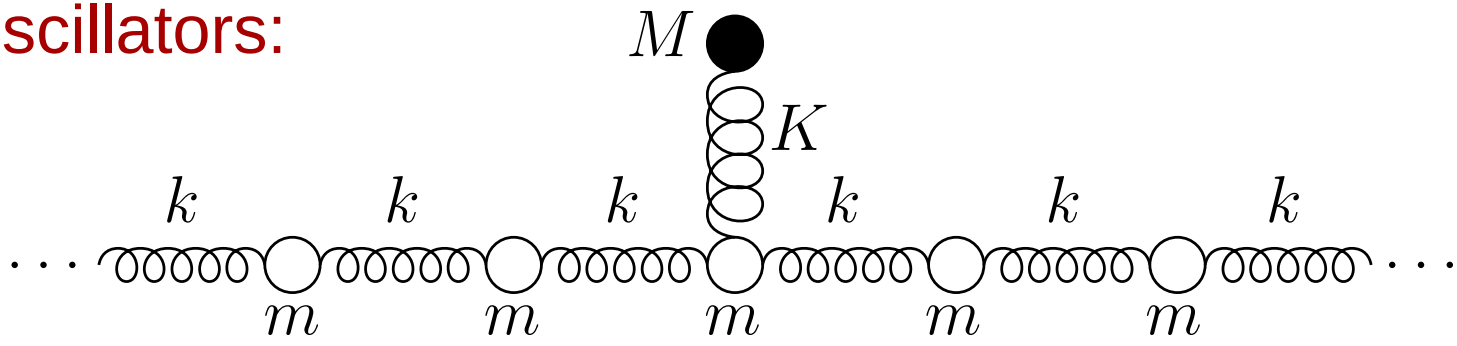
With simultaneous constraints of unitarity (quantum theory) and bounded speed of movement (special relativity), the best spatial search algorithms are found in the formalism of relativistic quantum mechanics.

Relativistic dispersion relation is satisfied by wave propagation but not by diffusion.

A Coupled Oscillator Model

Set of oscillators:



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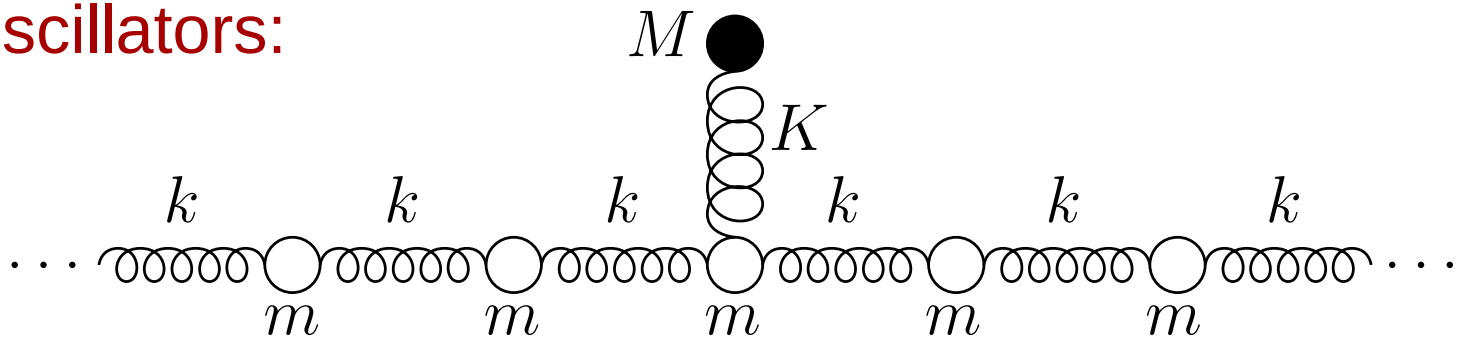
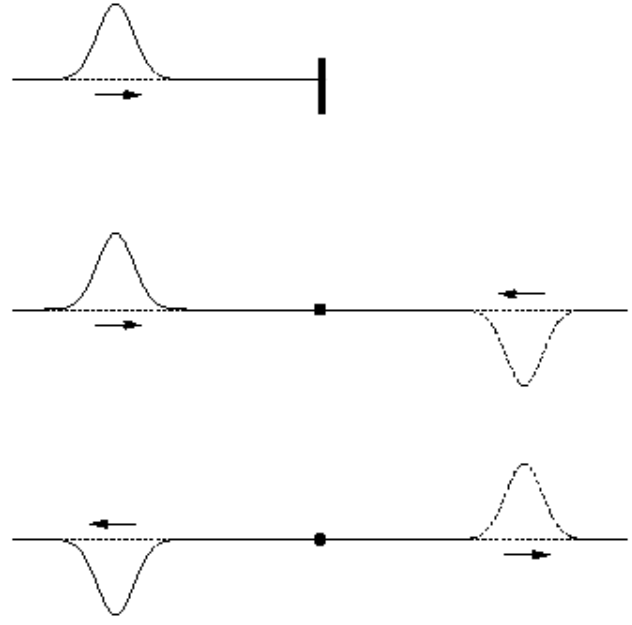


Reflection oracle:



Ingredients

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

Classical modes belong to the “decoherence free" subspace of the quantum modes.

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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.

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

Features

(a) The N identical oscillators may form a suitable network. A rigid scaffold would eliminate the free translation mode.

(b) The side branch oscillator acts as a storage cavity.

(c) The connection to the side branch produces both reflection and transmission (similar to a beam-splitter).

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(d) Tulsi's algorithm enhances amplitude amplification by alternating the mixing $R_{\pi+2\delta}|t\rangle\langle t| + |t_\perp\rangle\langle t_\perp|$ with the walk W.

Grover's algorithm corresponds to $\delta = 0$ and $W \rightarrow$ reflection about the average.

(e) The amplitude essentially evolves in a 3-dim subspace, formed by the cavity state, the target state coupled to the cavity, and an "averaged" non-target state.

(f) δ is optimised as a function of N and $\langle t|W|t\rangle$.
For a high-Q cavity, $\delta \approx \pi/2$.

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Challenge

Experimentally verify the physical criteria for high energy accummulation efficiency in the cavity, i.e. the resonance condition and the optimal parameters of Tulsi's algorithm.

References

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.

A. Tulsi, Faster Quantum Walk Algorithm for the Two-dimensional Spatial Search, Phys. Rev. A 78 (2008) 012310.

A. Patel, Efficient Energy Transport in Photosynthesis: Roles of Coherence and Entanglement, Proceedings of the Sympsium “75 Years of Quantum Entanglement”, AIP Conference Proceedings 1384 (2011), `arXiv.org:1104.1253`.

Thank You!