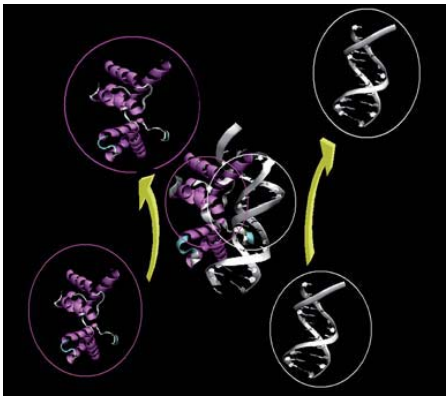
QUANTUM PHYSICS OF LIVING MATTER 2011



edited by
N. Poccia – A.R. Bishop – A. Bianconi

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Communications presented at the first Symposium on
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Contents

Introduction

This book reports the scientific communications presented at the first International Symposium on Quantum Physics of Living Matter held at Sapienza University of Rome on July 12-13, 2011 selected by the scientific program committee:
– Derek Abbot, The Univ. of Adelaide, Australia
– Ginestra Bianconi, Northeastern University, Boston, USA
– Paul C. W. Davies, Arizona State Univ., Arizona USA
– Vlatko Vedral, University of Singapore, Singapore
– Antonio Bianconi, Sapienza University of Rome, Dept. of Physics, Italy
– Alan R. Bishop, Los Alamos National Laboratory, Los Alamos, USA
– Nicola Poccia, Sapienza University of Rome, Dept. of Physics, Italy.

Preface

Quantum Physics of Living Matter

Nicola Poccia and Antonio Bianconi

While quantum effects are generally neglected in classical biophysics courses and in biophysical research, in the first ten years of this century new experimental and theoretical results, providing evidence for the role of quantum mechanics in living matter have been published in highly ranked science journals and are attracting a growing scientific interest. It is therefore the right time to organize a Symposium in this topic, to boost the research in this field bringing together active, scientists in the field and young participants.

Thank to advances in protein crystallography by synchrotron radiation and the capacity to control DNA polymerase reactions, many feature of the biological world such as proteomics and genomics have been thoroughly explored and at the molecular level explained. However besides the great amount of data covered by experimental investigations and theoretical modeling, at the present there is no unifying picture aiming to give some more quantitative definition of what is life and why is qualitatively different from the non living matter. The modern evolutionary synthesis, which marries Darwin's theory of natural selection with Mendel's genetics, have been developed the same period when quantum mechanics was founded and it is intriguing to ask if they were somewhat related. Quantum theory of condensed systems and quantum information theory are investigated in several complex materials and adaptive matter with several forms of competing interactions showing multiscale phase separation and basically unexpected functions. Living systems, however, are composed of large macromolecules of various types and they exist at high temperatures (about 300 Kelvin plus). Can any entanglement survive under such harsh conditions? It would seem unlikely that macroscopic thermal entanglement could exist at 300K, but it is very important to remember that living systems are not in equilibrium. They are in fact very much driven by their environments and continuously change in time. The technological convergence both for physi-

cists and biologists in the necessity of using experimental techniques, able to explore the micron-scale nano-scale spatial scale such as that provided by the most advanced synchrotron radiation sources and the femtosecond time scale such as that promised to be explored by free electron laser facilities, is a unique situation in the history of science and it could lead finally to common problems and questions in both these often separated community. Non equilibrium thermodynamic behavior and quantum macroscopic behavior are likely to be linked and they are both long standing concept relevant for physics, but due the recent findings and discussion on biological system, they are most probably in the next future to attract the attention of many biologists. Tremendous impressive experimental and theoretical advances in this new scientific field of "Quantum Physics of Living Matter" have been performed in these last years therefore we have planned the timeliness of the 2011 symposium in order to provide the possibility to discuss and to inform the new generation of young scientists about both theoretical aspects and new experiments with the aim to give the chance to grasp these seemingly disparate new concepts which are usually not considered together.

Quantum Photosynthesis

Experimental evidence has been reported for wavelike energy transfer thought quantum coherence in photosynthetic systems, that constitutes the first rigorous quantification of entanglement in a biological system. Two-dimensional electronic spectroscopy investigations of the FMO bacteriochlorophyll complex has given direct evidence for remarkably long-lived electronic quantum coherence playing an important part in energy transfer processes within this system [1]. Light-harvesting components of photosynthetic organisms are complex, coupled, many-body quantum systems, in which electronic coherence has recently been shown to survive for relatively long timescales, despite the decoherence effects of their environments [2-5]. Progress can also comes from x-ray techniques that can monitor structural changes in real time with 10-microsecond resolution occurring in photosynthetic reaction centers [6]. Protein conformational changes are in fact believed to participate in the function and regulation of photosynthetic Rhodobacter sphaeroides reaction center illuminated at room temperature before rapid freezing [7]. There is a growing interest on entanglement in many-body systems both from a fundamental and a technological point of view. This is not only a special problem related to the border of physics but it is a new feature emerging in biological systems that is attracting scientific interest.

Biological motors and Self-organized nanomachines.

Self-assembly is the process in which a system's components - be it molecules, polymers, colloids, or macroscopic particles - organize into ordered and/or functional structures without human intervention. The main challenge in self-assembly research is the ability to "program" the properties of the individual pieces such that they organize into a desired structure, in some cases exhibiting scale free properties [8-11]. This research aims to direct the assembly of nano-scale components into controlled and sophisticated structure has motivated intense efforts to develop assembly methods that mimic or exploit the recognition capabilities and interactions found in biological systems [12-13]. It has been reported a family of DNA tetrahedra, less than 10 nanometers on a side, that can self-assemble in seconds with near-quantitative yield of one diastereomer [14]. They can be connected by programmable DNA linkers. Moreover, it has been studied the three-dimensional tensegrity structures in which rigid bundles of DNA double helices resist compressive forces exerted by segments of single-stranded DNA that act as tension-bearing cables [15]. The melting behavior and breathing dynamics of double-stranded DNA as a function of nucleotide sequence is a topic of active study. Melting data for several DNA oligos have been used and Monte Carlo simulations have been applied to establish force constants for the 10 dinucleotide steps [16]. It is emerging that living organisms in fact are not just random collections of organic molecules and the quantum correlated dynamics and statistics emerge as essential features for their function.

Quantum information.

There is continuous information processing going on in the apparent bouncing around of molecules of life. Entanglement is emerging as a crucial term in explaining the stability of the DNA double helix [17] and in the avian compass of birds [18]. In particular, spectroscopic observations of a carotenoid–porphyrin–fullerene model system have been used to demonstrate that the lifetime of a photochemically formed radical pair is changed by application of very low magnetic fields such as that of the earth magnetic field [19]. The use of quantum dynamics as a tool in order to improve our comprehension of why living organisms have 4 nucleotide bases and 20 amino acids, as optimal solutions of the molecular assembly process will be discussed. The growing field of quantum biology deals with the question if living systems use non-trivial quantum effects to optimize some tasks.

Evolution and quantum mechanics

Recently the formal level of the mathematics of evolution has been developed showing that stimulating connections relates the evolutionary theory and quantum mechanics. There is evidence that the evolutionary process at the stationary state might undergo an interesting condensation phase transition in the universality class of a Bose-Einstein condensation [20]. Moreover path integrals describe the evolutionary dynamics on the extent that a certain population can be the results of many phylogenetic histories [21,22]. It is therefore clear that despite the fact that quantum mechanics rules the world at length scales many orders of magnitude below the size of Darwin's finches or Mendel's pea plants, quantum mechanics has a profound effect on the naturally selected world [23] and in this conference researchers will share with a broad scientific audience their results.

Quantum effects in living matter.

The problem of entanglement production during the evolution of a general quantum mechanical dissipative system is growing as a hot topic in the field [24]. Quantum critical fluctuations are mostly probably the source of entanglement in several condensed systems and a quantum critical behavior will be described with other real examples of decoherence process in quantum networks [25]. Moreover, quantum resonances have been found to rise the critical temperature of superfluid condensation such as Feshbach resonance in ultra cold gases and therefore have been proposed to be present also in other systems such as high temperature superconductors and living matter in order to avoid the lecherous effects due to temperature [26]. While is commonly accepted that quantum mechanics rules the world at length scales many orders of magnitude below the size of the macroscopic world, experimental results showing a correlation quantum mechanics in action in macroscopic world are appearing [27,28]. The symposium aim to start a series of conferences to establish connections between authors working in different and apparently unrelated field of biological science (chemical biology, reactive dynamics and genetics) with problems of quantum entanglement, quantum criticality, superfluidity, nanomaterials. Cross fertilization between these disciplines would have probably an impact on the new emerging field of quantum technologies inspired and emulating the biological world.

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SECTION I

I.1.
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Alan Bishop is an internationally recognized leader in condensed matter theory, statistical physics and nonlinear physics. He has made major contributions in the areas of solitons, quantum complexity, structural and magnetic transitions, collective excitations in low-dimensional organic and inorganic materials and complex electronic materials with strong spin-charge-lattice coupling. He is a Fellow of the American Physical Society, Fellow of the American Association for the Advancement of Science, a recipient of the Department of Energy's E.O. Lawrence Award, a Humboldt Senior Fellow, and a Laboratory Fellow.

Selected publications:

1. Olson Reichhardt CJ, Reichhardt C, Bishop AR (2007) Structure and fragmentation in colloidal artificial molecules and nuclei. *Eur. Phys. J. E - Soft Matter* 22, 11-15.
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In the post genome-sequencing capability explosion, the field of biology is now faced with new challenges, including understanding complex "systems" behavior, and the multiscale signatures now becoming evident through many remarkable advances in synthesis and spatio-temporal experimental probes. In particular, conformational deviations from the DNA canonical Watson-Crick double-helix template, are now clearly associated with essential biological processes – these are controllable pathways to the coding protected in the double-helix. This theme has a great similarity to the large-amplitude, local deviations from average structures which have been identified and assigned functionality over the last decade in a great variety of organic and inorganic non-biological materials – a topic of great interest for the community of scientists interested in stripes lattice textures in high temperature superconductors. We will focus our presentation on some of the functional relations now emerging in DNA.

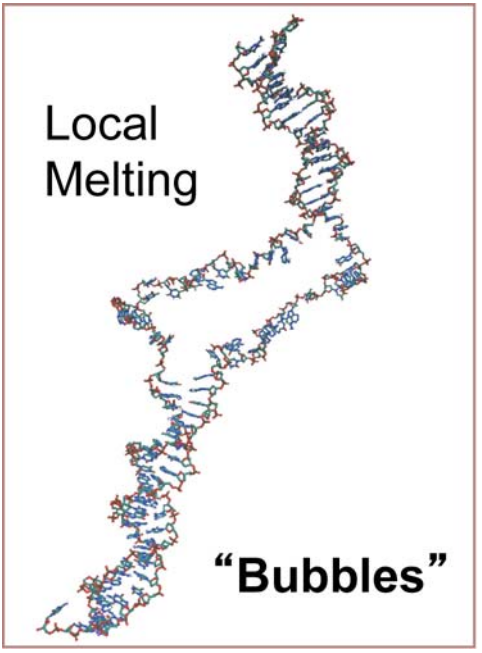

Figure 1: The long-lived transient openings in the double helix DNA with the formation of bubbles and local melting

Establishing the general and promoter-specific mechanistic features of gene transcription initiation requires improved understanding of the sequence-dependent structural/dynamic features of promoter DNA. Experimental data suggest that a spontaneous DNA strand separation at the transcriptional start site is likely to be a requirement for transcription initiation in several promoters. We describe our progress in using simulations of an effective nonlinear model to analyze the strand separation (bubble) dynamics of certain promoter DNA sequences. We argue that three criteria - bubble probability, bubble lifetime, and average strand separation - are needed to characterize bubble formation at the transcriptional start sites of a set of mammalian gene promoters. We observe that the most stable (longer lifetime) DNA openings do not necessarily coincide with the most probable openings and the highest average strand displacement, underscoring the advantages of accurate molecular dynamic simulations. The dynamic profiles of the tested mammalian promoters differ significantly in overall profile and bubble probability, but the transcriptional start site is typically distinguished by large (longer than 10 base pair) and long-lived transient openings in the double helix. In strong support of our simulation based arguments, our experimental transcription data demonstrate that an artificial bubble-containing DNA template is transcribed bidirectionally by human RNA polymerase alone, in the absence of any other transcription factors. We also describe recent extensions of our approach to very large DNA sequences, to effects of UV light, to effects of twist and torque, and to the potential effects of THz radiation on DNA conformations and cellular expressions.

Work performed with B. Alexandrov, and K. Rasmussen, and C. Nisoli (Los Alamos), and A. Usheva (Harvard Medical School).

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8. C. Nisoli and A. R. Bishop, PRL (2011).

I.2.
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Selected publications

1. Markus Arndt, Olaf Nairz, Julian Voss-Andreae, Claudia Keller, Gerbrand van der Zouw and Anton Zeilinger Wave-particle duality of C60 molecules Nature 401, 680-682 (1999).
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When we ask about the relevance of quantum physics in living matter we usually find two opposing answers: on the one hand it is evident that biology is built on chemistry and thus on quantum physics, too. On the other hand it is a matter of an ongoing debate what will be counted as a non-trivial quantum effect in biology [1].

Quantum physics has been known as one of the quantitatively best-confirmed models of nature for more than a century and it has become a central pillar in the building of modern physics and technologies. And yet, quantum predictions often seem to contradict our common sense when we try to understand the phenomena of 'quantum superposition' or 'quantum entanglement'. This is why the observation of either of the two phenomena over macroscopic distances or times is often listed as a key criterion for a 'non-trivial' quantum effect – also with regard to their relevance in living matter.

A series of recent experiments in Vienna has been targeted at generating spatial superpositions of isolated organic molecules [2]. By this we mean that under suitable circumstance even a single rather complex object may exist in two or more positions at the same time. This defies our everyday intuition and experience, which would regard the population of two remote places by the same thing as mutually exclusive and impossible.

Our recent quantum interference studies show that covalently bound complexes, composed of several hundred atoms, can be delocalized over micrometers and maintain quantum coherence in their center-of-mass motion over many milliseconds. This even holds when they are internally as hot as a 600 Kelvin, i.e. warmer than any living matter on Earth.

We find that the observation of quantum interference requires good shielding from all perturbations that might provide information about the molecular whereabouts. In general, this means that we need to properly prepare the initial molecular state and to subsequently protect it from all position-sensitive interactions with its environment.

We characterize the role of thermal photon emission as well as what vacuum is needed to keep the number of interactions on an acceptably small level, i.e. compatible with quantum behavior over a molecular flight distance of about one meter. Thermal and collisional decoherence, however, also easily explain why we cannot observe quantum superpositions of macroscopic bodies under ambient conditions over long distances in space and time.

While our coherence experiments already operate in the mass range of small proteins [2], I will also discuss what experimental developments are still required to also observe quantum delocalization with objects in the complexity class of

viruses – and which fundamental limitations one might expect or experimentally test along this way.

Although and because molecular interference is highly sensitive to all sorts of external perturbations it is still compatible with external force fields as long as these do not measure the particle's position. Quantum interferometry therefore allows us to pattern millimeter-sized molecular nanostructures in flight which are well suited to measure the *internal* molecular properties, such as polarizabilities, dipole moments or conformations even when the complexes are still in a *spatially quantum delocalized* state.

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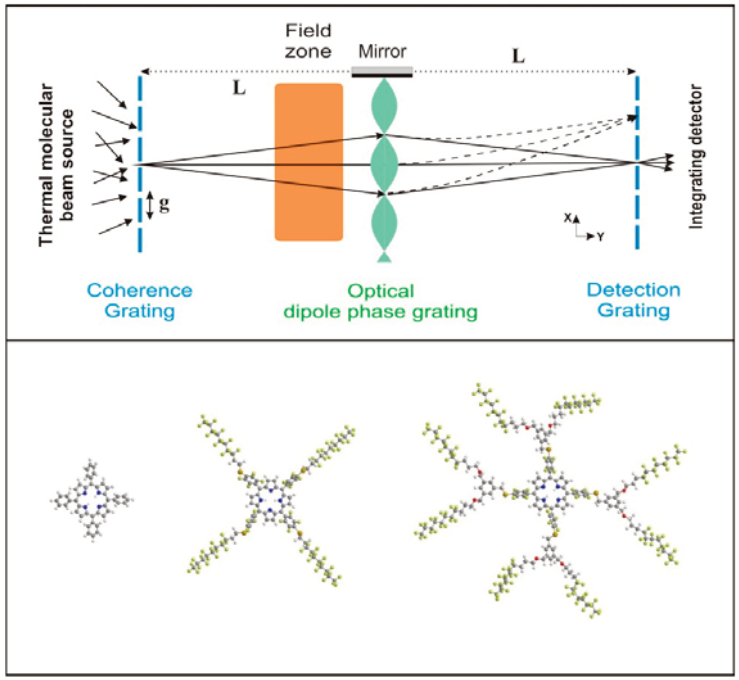

Figure 2: The Kapitza-Dirac-Talbot-Lau apparatus in Vienna is a near-field matter-wave interferometer. It is optimized for high-mass interference and quantum-enhanced metrology with organic molecules. The functionalized molecules for interference studies were synthesized by Jens Tüxen and Marcel Mayor, at the University of Basel.

I.3.

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Selected publications:

1. Quantum Algorithms and the Genetic Code, Pramana 56 (2001) 367-381, arXiv.org:quant-ph/0002037.
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6. Efficient Energy Transport in Photosynthesis: Roles of Coherence and Entanglement, Proceedings of the Symposium "75 Years of Quantum Entanglement: Foundations and Information, Theoretic Applications", SNBNCBS, Kolkata, AIP Conference Proceedings 1384 (2011), arXiv.org:1104.1253.

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

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 synthesized 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 viewpoint, we can analyze what has been optimized 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 realized in the framework of wave computation. Wave computation works in the same Hilbert space as quantum computation, and can provide coherent evolution without any entanglement.

The two have the same time and oracle complexity. Although wave computation requires larger spatial resources than quantum computation, it is far more robust against environmental disturbances. It is therefore useful in situations where spatial resources are cheap and quantum computation is fragile. Amplitude manipulation becomes energy manipulation in the wave language, which makes wave algorithms practical in a variety of problems including those in molecular biology.

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 neighbor 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 optimized, 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.

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4. A. Patel, Proceedings of the Symposium 75 Years of Quantum Entanglement, AIP Conference Proceedings 1384 (2011), arXiv.org:1104.1253

Figure 3: Photosynthesis in action

SECTION II

II.1.
E. Collini and G. D.Scholes

Coherent dynamics in energy migration at room temperature: Evidence for subtle quantum-mechanical strategies for energy transfer optimization

Electronic energy transfer (EET) is a process whereby the energy of absorbed light is transmitted between molecules. EET is a key photoinduced process for multichromophoric systems in biological photosynthesis, photovoltaic devices, photocatalysis, and sensors. For this reason in the recent years there have been many studies of EET phenomena and attempts to gain further insights into the mechanism of efficient EET. The pathways and timescales of EET for various multichromophoric systems ranging from photosynthetic complexes to conjugated polymers, to multibranched systems, are now well characterized in the frame of semiclassical theories (Förster model), in which the transfer rate can be calculated assuming incoherent quantum mechanical transitions.

However, the role of quantum coherences in determining the efficiency of energy transfer is still not well understood. This is especially true in the case of the so-called intermediate coupling, a particular regime for EET rising lot of interest because excitation moves in space, like in classical hopping mechanism, but still conserving quantum phase information.[1]

In this work we exploit two-dimensional photon echo experiments (2DPE) to observe quantum coherence dynamics in energy transfer on two evolutionarily related light-harvesting proteins isolated from marine cryptophyte algae. The data, recorded at room temperature, revealed exceptionally long-lasting excitation oscillations with distinct correlations and anti-correlations even at ambient temperature. These observations provide compelling evidence for quantum-coherent sharing of electronic excitation across the 5-nm-wide proteins under biologically relevant conditions, suggesting that distant molecules within the photosynthetic proteins are ‘wired’ together by quantum coherence for more efficient light-harvesting in cryptophyte marine algae. [2]

[1] E. Collini, G.D. Scholes, Science 323, 369-373 (2009)
[2] E. Collini, C.Y. Wong, KE. Wilk, P.M.G. Curmi, P. Brumer, G.D. Scholes, Nature 463, 644-648 (2010)

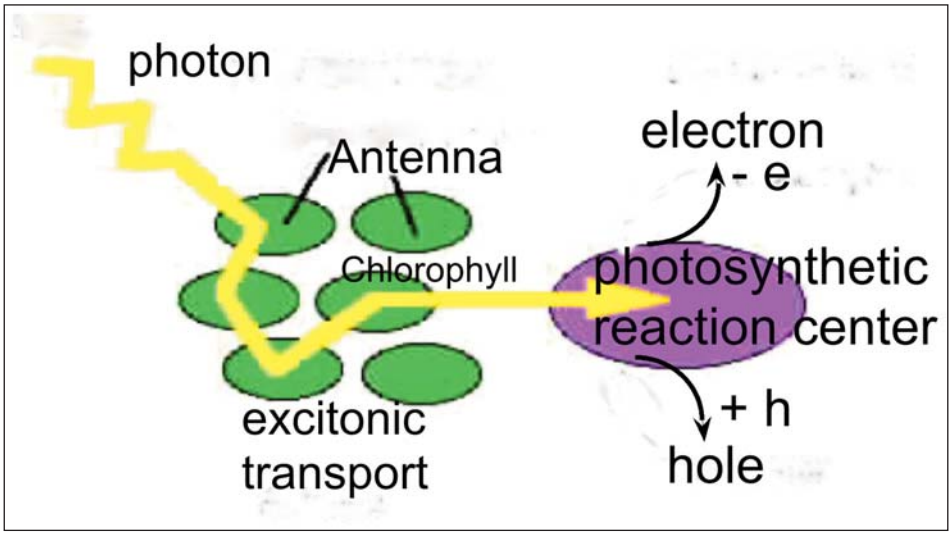

Figure 4: The photosynthetic system made of the antenna and the reaction centre, where the physical processes of photoabsorption, the exciton transfer in the antenna and the charge separation of electrons and holes in the reaction center take place.

II.2.
F. Caycedo

The role of light intensity adaptation in photosynthesis: Is quantumness really important to fulfill metabolic demands of purple bacteria?

Photosynthesis is arguably the fundamental process of life, since it enables photons to be converted into many-body excitations, and eventually fuel chemical reactions within a reaction center, to propel the first steps in the food chain. The precise nature of these dynamical processes—which lie at the interface between quantum and classical behavior—is a subject of current debate. In this talk, we focus on a striking recent empirical finding concerning an illumination-driven transition in the biomolecular membrane architecture of the purple bacteria *Rsp. photometricum*. Using stochastic realizations that describe a classical hopping, we are able to explain this surprising shift in preferred architectures of purple bacteria, that can be traced to the interplay between the excitation kinetics and the RC dynamics. The net effect is that the bacteria profit from efficient metabolism at low illumination intensities while using dissipation to avoid an oversupply of energy at high illumination intensities. This model allows us to explore the possibilities for photon-chemical conversion due to excitations transfer in the biomolecular membrane beyond classical hopping dynamics.

II. 3.
P. Faccioli

Dominant reaction pathways of biomolecules: from classical to quantum mechanical calculations

The investigation of the kinetics of rare thermally activated reactions by means of Molecular Dynamics (MD) simulations is limited by the fact that most of the computational time is invested to simulate the exploration of the (meta-) stable states. In this seminar, I will discuss how such a problem is rigorously bypassed in the recently developed Dominant Reaction Pathways (DRP) approach [1, 2, 3]. In particular, I will report on the first calculation of the dominant folding pathways of a peptide, based on ab-initio electronic structure calculations, rather than on an empirical force field [4]. Very recently, the DRP method has been upgraded to systematically account for the quantum corrections to the diffusive motion of the atomic nuclei [5], up to order . We have applied this method to study quantum delocalization effects in the conformational transitions of a peptide. We found that such quantum corrections are quite large and give raise to counter-intuitive effects.

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II.4.

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Effects of the measuring light on the photochemistry of the bacterial photosynthetic Reaction Centre protein from *Rhodobacter sphaeroides* purple bacteria

Since 1980s the bacterial Reaction Centre (RC) protein has become a reference model in the study of the interactions of quinone cofactors with photosynthetic electron transfer complexes. In these studies the RC functionality was investigated through flash-induced absorption changes (known as *flash photolysis* experiments, Figure 1 top) where the state of the primary donor (P) is probed by a continuous monitoring (i.e. measuring) beam, while the electron transfer is triggered by a short saturating light pulse (e.g. laser) generating a P^+X^- charge-separate state (X are cofactors involved in the RC electron transfer chain, such as bacteriopheophytin and ubiquinones at Q_A, Q_B sites). The single-beam set-up implies the use as reference of the transmittance measured before the light pulse. Implicit in the analysis of these data is the assumption that the measuring beam does not significantly influence the protein photochemistry. At variance, the monitoring beam is actinic in nature at almost all the wavelengths suitable for probing the RC functionality. In this context, a detailed analytical modeling of the time evolution of neutral and charge-separated RC species has been performed, based on photolysis experimental data. The measuring light induces a first order growth of the charge-separated state up to a steady-state depending on the light intensity and the occupation of the secondary quinone (Q_B) site (Figure 1 bottom). The intervention of a laser pulse pumps all the RCs in the $P^+Q_A^-$ or $P^+Q_AQ_B^-$ states. The following relaxation kinetics from such states (*charge recombination*) is still affected by the measuring beam (Figure 2). The kinetics of charge recombination measured in native RC preparations with the QB site partially occupied are two-exponential. The rate constants of both fast and slow phases depend linearly on the measuring beam intensity, while their relative weights depend not only on the effective RC fractions with quinone unbound/bound to QB site but also on the measuring light intensity itself. Our analytical model provides full awareness of the perturbation induced by the measuring beam in photolysis measurements on RC samples, with interesting opportunities: (i) obtaining reliable estimates of the Q_B site occupancy, very significant for understanding the RC photochemistry; (ii) the possibility of artificially populate the $P^+Q_A^-$ state from the $P^+Q_B^-$ one by means of a suitable monitoring light, with the effect of "quenching" the slow phase in charge recombination experiments.

SECTION III

III.1.

A. De Ninno and A. Congiu Castellano

Effect of Weak Magnetic Field on Glutamic Acid

A wide literature is available on the effects of weak Extremely Low Frequency Electromagnetic Fields (ELF-EMF) on the biochemical reactions, nevertheless the physical nature of these effects is largely unknown. The main conundrum is the mismatch between the tiny amount of the energy delivered by the perturbation and the response of the system.

We have measured the influence of ELF-EMF on glutamic acid solutions in water through FTIR-ATR technique. Samples have been exposed for 10, 20 or 30 minutes to a weak EMF generated by Helmoltz coils and then placed into the spectrometer. After the exposure solutions having a pH lower than the isoelectric point show a shift toward the de-protonation of the carboxylic group, while solutions having a pH greater than the isoelectric point show the de-protonation of the residual amine group. Moreover, at low pH values, we have also observed a shift of the band of the amine which can be related to a change of the degree of hydrogen bonding.

The effect lasts for minutes after the exposure before the native configuration is restored. Spectra modifications have been observed after each independent exposure to EMF, the same effect has been observed by varying the frequencies in the range 0-7 KHz, thus the hypothesis of the existence of a resonant frequency, elsewhere proposed cannot be supported by this study. The most surprising feature of this effect is the existence of long life perturbation. This implies a high degree of correlation among a great number of molecules. The existence of a defined phase relationship among the molecules concerned can account for a degree of coupling among molecules that is stronger than that with the environment. Similar examples to those provided by our study may be found in the literature. It has been shown that long-lasting electronic quantum coherence plays an important part in energy transfer processes in biological systems, thereby explaining the extreme energetic efficiency of living organisms.

III.2.

Michela Fratini, Stefano Iotti, Giovanna Farruggia, Alessia Cedola, Valentina Trapani, Inna Bukreeva, Andrea Notargiacomo, Lucia Mastrototaro, Chiara Marraccini, Andrea Sorrentino, Ian McNulty, Stefan Vogt, Daniel Legnini, Alessandra Gianoncelli, Jeanette A M Maier, Federica I Wolf & Stefano Lagomarsino

Determination of Mg concentration map in whole cells by nanoprobe techniques

Magnesium (Mg referring to both bound and free form of the cation) plays crucial structural and regulatory roles within all cells. Intracellular Mg is very abundant and widely distributed; its content is finely tuned through plasma membrane transport, as well as buffering and compartmentalization in intracellular organelles, including mitochondria. Moreover, the release of Mg from mitochondria might play a key role in cell survival/death. Despite recent efforts in applying new live imaging techniques to the field of magnesium research,an accurate characterization of Mg distribution in the cellular environment is still lacking. We present a novel methodological approach which allowed to map the intracellular concentration of Mg for the first time. Recent improvements in third-generation synchrotron X-ray sources and in X-ray focusing have led to X-ray micro- and nano-probes with high sensitivity and spatial resolution, which find widespread applications, not least in cellular biology. In particular, scanning fluorescence X-ray microscopy (SFXM) is a microanalytical technique ideally suited for mapping elemental distribution in whole cells or tissue sections.SFXM may give quantitative information on elemental concentration, as opposed to content, provided it is applied to sample sections or slices of known thickness, such as those used for electron microscopy. This strongly limits the amount of achievable information: measuring a single section does not reveal the distribution of the target element throughout the whole cell. We develop a novel experimental approach that combines scanning fluorescence X-ray microscopy with atomic force microscopy to determine the intracellular concentration of a light element with high spatial resolution. We demonstrate that accurate normalization of the fluorescence signal by sample thickness is necessary to obtain quantitative information on elemental concentration, as opposed to content, in whole cells. We applied this technique to derive the first concentration map of magnesium in whole dehydrated cell.

III.3.

Gabriele Ciasca, Gaetano Campi, Anna Battisti, Marina Rodio, Nicola Poccia, Alessandro Ricci, Alexander Tenenbaum and Antonio Bianconi

Temperature dependent conformatioonal landscape of intrinsically disordered proteins

The thermal collapse of intrinsically disordered proteins (IDPs) has recently attracted much attention due to its general implication on several fundamental aspects of protein folding. Here, we present an extensive small-angle X-ray scattering study of the thermal behavior of the tau protein, an IDP which play a kay role in the development of many neurodegenerative deseases, like Alzheimer's desease. Our results indicate that the tau protein undergoes a strong thermal collapse, with a reduction in its radius of gyration Rg of about 19% when the temperature is increased in the range 293 K -333 K. This collapse is partially irreversible, as shown by a recovery of only 1/3 of the collapse when the temperature is decreased in the same range [2]. Moreover, as the temperature increases, the size distribution of the protein becomes narrower, suggesting that the thermal collapse phenomenon induces a reduction in the conformational space sampling.The mechanism behind the thermal collapse is currently under debate, and a prominent role of secondary structures has been proposed. We have discussed this hypothesis using data extracted from a recent Molecular Dynamics simulation of tau, and found indeed that the decrease of Rg is coupled by an increase of secondary structures entailing H-bonds.

SECTION IV

IV.1.
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He is an international recognized leader in quantum theory of information. He is professor of mechanical engineering at the Massachusetts Institute of Technology. He is principal investigator at the MIT Research Laboratory of Electronics, and directs the Center for Extreme Quantum Information Theory. His research area is the interplay of information with complex systems, especially quantum systems. He has performed seminal work in the fields of quantum computation and quantum communication, including proposing the first technologically feasible design for a quantum computer, demonstrating the viability of quantum analog computation, proving quantum analogs of Shannon's noisy channel theorem, and designing novel methods for quantum error correction and noise reduction.

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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 talk 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 complexity that is `just right' for attaining maximum efficiency. The functional purpose of the convergence of time scales is hard to establish, 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 [1]. We applied this technique to the Fenna-Matthews-Olson complex (FMO), a seven-chromophore energy transport complex in green sulphur bacteria [2]. 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. Moreover, the efficiency of transport was shown in [1-2] to be a function of a single underlying parameter that is lin-

ear in the various timescales themselves. The purpose of this talk is to give a heuristic but quantitative derivation for how convergence of timescales yields robust transport.

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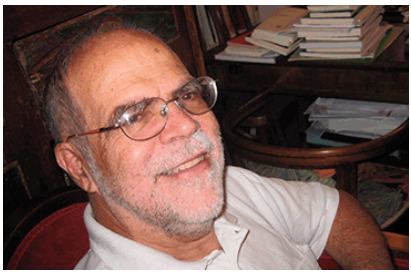
THE ORGANIZERS AND THE SCIENTIFIC COMMITTEE



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Antonio Bianconi investigate quantum phenomena in complex matter. He has developed new experimental methods using synchrotron radiation for the study of complex systems: proteins, high temperature superconductors, valence fluctuation materials, transition metal oxides, amorphous systems, surface layers, catalysts, functional materials. He has introduced the XANES spectroscopy and the XEOL method, In high temperature superconductors he has shown that doped holes in cuprates are in the oxygen orbital by Cu L23 XANES, he has introduced the lattice stripes scenario and has proposed the quantum mechanism of shape resonance in superconducting gaps for the amplification of the critical temperature. He is author of more than 320 papers in international journals, and 7 books. Now works on structural fluctuations by developing the use scanning nano x-ray diffraction for imaging lattice textures in out-of-equilibrium systems, in photostimulated lattice manipulation and conformational fluctuations in intrinsically disordered proteins.

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Selected publications:

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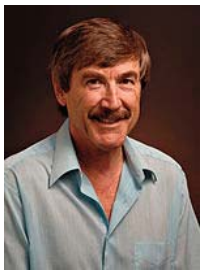

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