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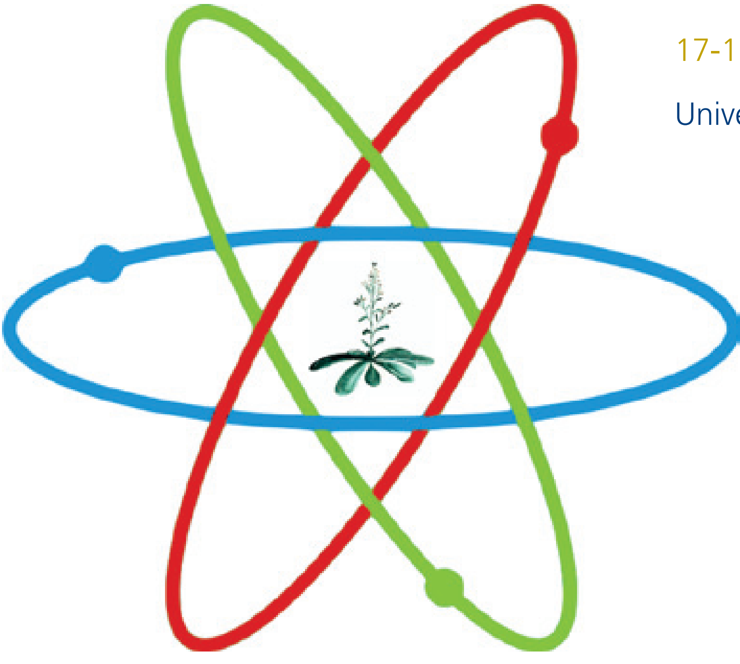
Quantum Biology: Current Status and Opportunities



17-18 September 2012

University of Surrey, UK

Programme

MILES Models and Mathematics in Life and Social Sciences

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Quantum Biology: Current Status and Opportunities

Introduction

Sixty years ago, Erwin Schrödinger, one of the founding fathers of quantum mechanics, puzzled over one of deepest mysteries: what makes genes so durable that they can be passed down through hundreds of generations virtually unchanged? To provide an answer, Schrödinger looked towards the science that he helped to build. In his book, "What is Life?" (first published in 1944), he suggested that life was unique in that some of its properties are generated, not by the familiar statistical laws of classical science, but by the strange and counterintuitive rules of quantum mechanics.

Although "What is Life" was influential in stimulating interest in the fundamental features of life, by-and-large Schrödinger's extraordinary proposal of quantum mechanics playing a key role was ignored by twentieth century biologists. But in the second decade of the twenty-first century, ignoring Schrödinger's bold proposal is no longer an option. Physicists have been intrigued to discover quantum effects in living systems; and biologists have been pulled, often reluctantly, into the quantum arena. Experiments performed by eminent scientists at some of the most reputable laboratories in the world have demonstrated quantum weirdness in such biologically-fundamental phenomena as photosynthesis and enzyme action. The strange rules of quantum mechanics have also been implicated in bird migration, our sense of smell, the origin of life and even the way our brain works.

This workshop on Quantum Biology will bring together eminent international researchers who have made landmark advances in this field. By bringing together both biologists and physicists we hope that this workshop will stimulate new interdisciplinary approaches to explore the role of quantum mechanics in biology.

Organisers:
Professor Johnjoe McFadden, Faculty of Health and Medical Sciences, University of Surey
Professor Jim Al-Khalili, Faculty of Engineering and Physical Sciences, University of Surrey
Professor Vlatko Vedral, University of Oxford

Programme of Talks

Day 1 Monday 17 September

Wates House, Treetops Room

09.00	Registration and coffee
0925	Welcome
Session 1	**Chair: Jim Al-Khalili**
0930	Johnjoe McFadden **Quantum mechanics, stochasticity and biology**
1015	Paul Davies **Quantum epigenetics**
1100	*Coffee*
Session 2	**Chair: Nigel Scrutton**
1130	Jim Al-Khalili **Quantum tunneling models of genetic mutations**
1215	**Short talks** Janet Anders – *"Contribution of quantum tunnelling events in chemical rates"* Karoline Wiesner – *"Studying biology with quantum Occam's razor"*
1300	*Lunch*
1355	Welcome from President and Vice Chancellor of Surrey, Professor Sir Christopher Snowden
Session 3	**Chair: Vlatko Vedral**
1400	Greg Scholes **Evolution, speciation, and coherence in the light harvesting proteins of photosynthetic algae**

1445	Alexandra Olaya-Castro **Quantum phononics in biology**
1530	*Coffee and Posters*
Session 4	**Chair: Thorsten Ritz**
1600	Greg Engel **Design principles behind long-lived quantum coherence**
1645	**Short talks** Ahsan Nazir – *"Strong coupling master equations for excitonic energy transfer dynamics"* Libby Heaney – *"Quantum coherent contributions to electron transport in respiratory complex I"*
1730	**Drinks Reception** (Wates House)
1900	**Workshop Dinner** (The Withies Inn, Compton village) Transport organised from the University at 1900 (University Library)

Programme of Talks

Day 2 Tuesday 18 September

Wates House, Treetops Room

0830	*Coffee*
Session 5	**Chair: Paul Davies**
0900	Thorsten Ritz **A biological compass built on coherent quantum reactions: Design principles and supporting evidence**
0945	Jennifer Brookes **Can the nose smell quantized properties of odorant molecules in olfaction?**
1030	*Coffee*
Session 6	**Chair: Greg Scholes**
1100	Nigel Scrutton **Quantum tunneling and dynamics in enzyme catalysed H-transfer**
1145	**Short talks** Sam Hay – *"Quantum selection of enzyme substrates?"* Martin Robert – *"Is the apparent emergent spacio-temporal and multi-scale organization of living systems connected to quantum coherence?"* Iannis Koninis – *"Quantum Dynamics of the Chemical Compass"*
1245	*Lunch*
Session 7	**Chair: Johnjoe McFadden**
1345	Sandu Popescu **What is quantum in quantum biology?**

1430 Vlatko Vedral
Quantum thermodynamics of electron transport

1515 *Coffee*

Session 8

1545 **General Discussion / Future Directions**
To be led by Vlatko Vedral

1700 **End of day 2**

Keynote Speakers

Dr Alexandra **Olaya-Castro**, University College, London, UK

Quantum phononics in biology

I will discuss how energy steering in some molecular components of living organisms may take advantage of non-classical behaviour of their vibrational environments. In particular, I will show how coherent interactions between electronic degrees of freedom and high-energy vibrations together with decoherence induced by a thermal background, guarantees that optimal energy transfer between chromophores is accompanied by optimal non-classical behaviour of the vibrations promoting transport.

Alexandra became a Lecturer in the Department of Physics and Astronomy of University College London in 2011 while still holding an EPSRC Research Fellowship which she obtained in 2008. She finishes her doctorate in Physics at the University of Oxford in 2005 and subsequently held a Junior Research Fellowship at Trinity College, Oxford until 2008. Her main research subject concerns quantum dynamics of systems embedded in structured environments. She is currently investigating the possible roles of quantum phenomena in the function of molecular components of living organisms.

Professor Paul **Davies**, Arizona State University, USA

Quantum epigenetics

Biological organisms process information in two ways: genetically and epigenetically. The former is digital, the latter is mainly analogue. The source of genetic information can be identified with a physical structure – DNA – but epigenetic information processing has no identifiable source: it is nonlocal and systemic, and implemented by peptides rather than nucleic acids. Chromatin represents the intersection of the realm of genetic and epigenetic information flows. It is a mesoscopic, partiallyordered, highly-dynamic, information-rich medium that is ill-understood either theoretically or experimentally. In the words of the late Jon Widom, textbook discussions of chromatin are mostly "make-believe". Quantum mechanics undoubtedly plays a crucial role in chromatin architecture and dynamics, but understanding it is daunting due to the complexity. It seems likely that evolution will have selected certain peptide sequence motifs on account of their quantum efficacy in this regard. In my lecture I will describe a new experimental project at Arizona State University to measure the quantum tunnelling current differences through amino acids – part of a single-molecule proteomics programme – that may assist in identifying the said motifs.

Paul Davies is a British-born theoretical physicist, cosmologist, astrobiologist and best-selling author. He is Regents' Professor and Director of Beyond: Center for Fundamental Concepts in Science, at Arizona State University, where he is also Co-Director of the Cosmology Initiative and Principal Investigator of the Center for the Convergence of Physical Science and Cancer Biology. Prior to his move to the USA in 2006, he helped create the Australian Centre for Astrobiology in Sydney. His research has focused mainly on the theory of quantum fields in curved spacetime, with applications to black holes and the inflationary phase *of the early universe. His current research includes computational models of the origin of life and an investigation of the deep evolutionary roots of cancer. Davies has written about 30 books, many for the general public. His most recent is The Eerie Silence: are we alone in the universe? In 1995 he was awarded the Templeton Prize for his work on the deeper meaning of science. He was also awarded the Faraday Prize by The Royal Society, the Kelvin Medal by the UK Institute of Physics, the 2011 Robinson Cosmology Prize, and many book awards, as well as three honorary degrees. In June 2007 he was named a Member of the Order of Australia in the Queen's birthday honours list and in December 2011 he was presented with the Bicentenary Medal of Chile. The asteroid 1992 OG was renamed (6870) Pauldavies in recognition of his work on cosmic impacts.*

Professor Greg D. **Scholes**, Department of Chemistry, Institute for Optical Sciences and Centre for Quantum Information and Quantum Control, University of Toronto, Canada

Evolution, speciation, and coherence in the light harvesting proteins of photosynthetic algae

In this talk the interplay between evolutionary ecology and quantum mechanical effects in light harvesting will be discussed with respect to how nature has found highly efficient and robust lightharvesting machinery. The antenna proteins of cryptophyte algae are used to illustrate the evolutionary diversification process, both on a structural and consequently a photophysical level. Experimentally, two-dimensional electronic spectroscopy was able to show the existence of quantum coherence in the response of light-harvesting proteins to illumination. The implications of quantum mechanical effects in the optimization of light harvesting and what that means for the design of artificial light-harvesting devices will be discussed.

Greg Scholes is the D.J. LeRoy Distinguished Professor at the University of Toronto in the Department of Chemistry. He undertook his PhD studies at the University of Melbourne, then held postdoctoral positions at Imperial College London as a Ramsay Memorial research fellow (Prof David Phillips) and at the University of California, Berkeley (Prof Graham Fleming). His present research concerns understanding light-initiated dynamics in systems ranging from semiconductor nanocrystals to conjugated polymers to photosynthetic light-harvesting proteins. Recent awards include the 2011 Sackler Prize in Chemical Physics from Tel Aviv University and election to the Academy of Science, Royal Society of Canada in 2009. Dr. Scholes serves on the editorial advisory board of several journals, as an Editorial Advisor for New Journal of Physics and is a Senior Editor for the Journal of Physical Chemistry Letters

Keynote Speakers

Professor Nigel **Scrutton**, University of Manchester, UK

Quantum tunneling and dynamics in enzyme catalysed H-transfer

Kinetic isotope effects (KIEs) are sensitive probes of the mechanisms of H-transfer in enzymes. We have exploited the dependence of KIEs as a function of temperature and pressure as probes of quantum mechanical tunneling and dynamics in enzyme catalysed reactions. Using a variety of enzyme systems I will present evidence for quantum tunneling in enzyme systems and the potential role of barrier compression in these reactions. Experimental studies exploiting KIE measurements are supported by computational simulations of the transfer chemistry using hybrid QM/MM and other computational methods. These studies indicate that quantum tunneling of hydrogen is widespread in biological systems and is potentially assisted by fast promoting motions. These fast promoting motions are conjectured to compress the free energy barrier leading to enhanced wavefunction overlap and thus a higher probability of tunneling.

Nigel received a degree in Biochemistry and was awarded the Robson prize from the University of London, King's College (1985). He gained his PhD (1988) as a Benefactors' Scholar (St John's College) from the University of Cambridge and his ScD (2003) degree also from Cambridge. At Cambridge he was awarded the Henry Humphreys research prize (1989), held a Royal Commission for the Exhibition of 1851 Research Fellowship (1988-91), a St John's College Research Fellowship (1989-92) Enzymology at the University of Manchester (2005), BBSRC Professorial Research Fellow (2006-2011) and Associate Dean for Research (2008-2010). He is currently Director of the Manchester Interdisciplinary Biocentre (2010 - present) and holds an EPSRC Established Career Fellowship in Catalysis (2012-2017). He is recipient of the Biochemical Society Colworth and a Royal Society University Research Fellowship (1991-1999). He also held a Fellowship and was Director of Studies for Biology at Churchill College, University of Cambridge (1992-95). In 1995 he moved to the University of Leicester as Royal Society University Research Fellow, where he later became Lister Institute Research Professor of Biochemistry (1999-2004) and Professor of Biochemistry (1999-2005). He was subsequently appointed Professor of Molecular Medal, the Royal Society of Chemistry Charmian Medal, the RSC Rita and John Cornforth Award and a Royal Society Wolfson Research Merit Award.

Professor Thorsten **Ritz**, UC Irvine, USA

A biological compass built on coherent quantum reactions: Design principles and supporting evidence

Abstract not supplied.

Thorsten Ritz is a biophysicist interested in the role of quantum mechanics in biological systems, ranging from photosynthetic light harvesting systems to sensory cells. He has championed the idea that a quantum mechanical reaction may lie at the heart of the magnetic compass of birds and other animals.

Straddling and often breaking the barriers between theory and experiment and physics and biology, he has worked with biologists to provide the first experimental evidence supporting a quantum-based compass in birds. He is currently an associate professor of physics and astronomy at the University of California, Irvine. His work has received national and international recognition, including awards from the Royal Institute of Navigation (UK), Institute of Physics (UK), American Physical Society, Alfred P. Sloan Foundation, and the Research Cooperation.

Dr Jennifer **Brookes**, Harvard University, USA

Can the nose smell quantized properties of odorant molecules in olfaction?

The machinery with which we smell odorants are biologically well understood (Buck, 1991). What is lacking in the field of olfaction is elucidation towards how these machines run. In particular, how does the smell molecule communicate to the receptor? It is widely believed that 'lock & key' theory describes smell response yet at close examination it is insufficient as a theory to describe expectations and results when one molecule does or doesn't affect a receptor. The classical mechanics paradigm is insufficient. Turin proposes a signalling mechanism which determines smell molecules by quantum mechanics (Turin 1996), where a form of inelastic electron tunnelling is a probe used by the receptor to recognize an appropriate molecule. Investigation of this mechanism shows it to be physically viable (Brookes,et al, 2007), and it proves useful to examine as quantitative measure of scent. Perhaps quantum mechanics is a more appropriate paradigm within which to model olfactory signalling. We explore ideas where shape and quanta of the odorant molecules are important were the 'fit' of molecules combined with a quantal description of the running of the machinery seems to be sufficient and necessary in the process. We investigate the theory and the possibilities.

Brookes, J.C, Hartoutsiou, F, Horsfield, A.P and Stoneham, A.M. (2007). Physical Review Letters 98, no. 3 038101
Buck, L. (1991) Cell, 65, no.1 (4): 175-187.
Turin, L. (1996) Chemical Sences 21, no 6. 773-791

I am a Sir Henry Fellow supported by the Wellcome Trust, UK, hosted by the London Centre for Nanotechnology (LCN) at University College London (UCL). I was awarded the Sir Henry Wellcome Post-doctoral Fellowship in 2009 for work towards the understanding the recognition mechanisms between enigmatic molecules such as odorants and their receptor proteins. Since then I spent a year at Massachusetts Institute of Technology hosted by the Zhang Lab and I am currently a visiting research scholar at the Aspuru-Guzik lab at Harvard. I commenced the 4 year's fellowship in October 2009 following a 1 year research assistant position to Marshall Stoneham FRS at the LCN, UCL. The year before I completed my thesis, also at UCL, under the supervision of Marshall Stoneham FRS, and Andrew Horsfield. My research interests are in quantum processes in biology, molecular simulations (classical dynamics and ab initio), data analysis and signaling, and nanotechnology with medical applications.

Keynote Speakers

Professor Jim **Al-Khalili**, University of Surrey, UK
Quantum tunnelling models of genetic mutations

Quantum tunnelling is thought to be involved in a wide range of biochemical processes including photosynthesis, respiration, mutation and protein folding. For instance, enzymes that establish the proton gradient that drives the F1-ATPase are thought to couple proton transport to electron tunnelling. Indeed both electron and proton tunnelling are considered by many to be the missing ingredients that account for the ability of enzymes to massively accelerate chemical reaction rates. Quantum tunnelling is also thought to be involved in photosynthesis and protein folding. And it may be fundamental to the evolution of life on Earth.

Watson and Crick first suggested that DNA base tautomerisation – a chemical euphemism for proton tunnelling - within the double helix, is responsible for mutations. This mechanism was further explored fin the early 60s by the Swedish physicist, Per-Olov Löwdin [1]. Since then, much effort has been focussed on exploring this phenomenon [2] mainly by quantum chemists. But, remarkably, we still have no definitive answer to the question of whether quantum tunnelling plays a role in genetic mutations alongside other better established and understood mechanisms. This talk will review some of the effort in the field as well as show some preliminary results from the work being carried out by the Surrey physics group using time-dependent density matrix dynamics by solving the Liouville-von Neumann equation for open quantum systems [3] for proton tunnelling in an asymmetric double potential well to model H-bonds between base pairs in DNA, including the effects of dissipation of quantum coherence via coupling to an external heat bath.

[1] P-O Löwdin, Rev. Mod. Phys. 35 (1963) 724
[2] E S Kryachko and J R Sabin, Int. J Quant. Chem. 91 (2003) 695
[3] C. Scheurer and P. Saalfrank, J. Chem. Phys. 104 (1996) 2869

Jim Al-Khalili OBE is professor of physics at the University of Surrey where he also holds a chair in the Public Engagement in Science. He gained his PhD in theoretical nuclear physics from Surrey in 1989 before spending time at University College London. In 1991, he returned to the Surrey nuclear theory group, first as a postdoc then as a tenured lecturer (assistant professor). He also held a five-year EPSRC Advanced Research Fellowship (1994-99). He has spent time at TRIUMF Lab in Vancouver and the Niels Bohr Institute in Copenhagen. He has published widely on nuclear reaction theory and few-body quantum scattering models to elucidate the structure of exotic, neutron-rich (halo) nuclei. He is also active as a science communicator, author and broadcaster and has written a number of popular science books. Quantum biology is a relatively new area of interest for him with the aim of applying quantum models developed in nuclear physics to microbiology. He is also currently writing a popular science book on this new field.

Professor Johnjoe **McFadden**, University of Surrey, UK

Quantum mechanics, stochasticity and biology

Quantum mechanics and molecular biology were the two revolutionary scientific disciplines that grew out of the twentieth century. Quantum biology can be said to have been initiated by a physicist, Erwin Schrödinger, in his lecture, essay and book entitled "What in Life" (published in 1944) in which he proposed that that heredity was based on non-trivial aspects of quantum mechanics. The book was very influential to molecular biology pioneers, such as James Watson and Francis Crick, who speculated that quantum tunnelling may be the driver for mutation in DNA. This idea was given a firm theoretical foundation by the Swedish physicist Per-Olov Löwdin in the 1960's; but thereafter the field of quantum biology largely languished; albeit with occasional bursts of interest, such as the speculation that consciousness is based on quantum mechanics, stimulated by Roger Penrose's book, "The Emperor's New Mind" in 1989. However, the twenty-first century has seen a revival of quantum biology with the arrival of new experimental evidence of quantum mechanical effects in a range of biological phenomena such as photosynthesis and enzyme action. In this talk I will provide an introduction to quantum biology, returning to Schrödinger's original insight that stochastic quantum phenomena may be found in biological processes that involve very numbers of molecules. I will review the kinds of biological phenomena that may be subject to these quantum stochastic effects and present some recent experimental evidence that proton tunnelling is involved in mutation.

Johnjoe McFadden is Professor of Molecular Genetics at the University of Surrey. He graduated from the University of London and went on to Imperial College to study for his PhD plant virus genetics. Since then his main research work has focussed on elucidating virulence mechanisms and pathways of human pathogens, particularly the agents that cause tuberculosis and meningitis. In recent years his focus has shifted to systemsbased approaches to investigate infectious disease, for instance, constructing the first genome-scale metabolic networks for Mycobacterium tuberculosis in 2007 and the Neisseria meningitides in 2011. Johnjoe McFadden has maintained a strong interest in quantum biology, publishing a theoretical paper with Jim Al-Khalili in 1999 on the role of quantum mechanics in mutation; and then writing a popular science book, Quantum Evolution in 2000 (published by HarperCollins in the UK and by WW Norton in the USA) exploring the role of quantum mechanics in biology. As well as his mainstream work, McFadden writes popular science articles for newspapers in the UK and internationally.

Keynote Speakers

Professor Vlatko **Vedral**, University of Oxford, UK
Quantum thermodynamics of electron transport

Obtaining the free energy profile in various electron transport problems is crucial for understanding if quantum coherence plays any role in transport. I discuss a method arising from the Jarzynski equality (non-equilibrium thermodynamics) to show how the free energy profile could be estimated from the repeated measurements of the electron two-point correlation function.

Vlatko Vedral is a professor of quantum information at the University of Oxford (Fellowship of Wolfson College) and a professor of physics at the Centre for Quantum Technologies at the National University of Singapore. He is best known for his research on the theory of quantum entanglement and quantum information. He has published over 190 research papers in quantum mechanics and quantum information and was awarded the Royal Society Wolfson Research Merit Award in 2007 and the World Scientific Medal and Prize in 2009. At some point in his career he has held permanent positions at Imperial College and Leeds University, visiting professorships in Vienna and at Perimeter Institute in Canada. He is the author of several books, including the popular science book Decoding Reality.

Professor Greg **Engel**, University of California, USA
Design principles behind long-lived quantum coherence

Photosynthetic antenna complexes operate with near unity efficiency and steer excitonic motion with exquisite precision. Optimized by evolution, these biological systems display intriguing behaviors including coherent energy transfer and protection of long-lived quantum coherence. The interaction between the chlorophyll molecules and vibrations (thermal and driven) in both the chromophore and in the protein environment drive these dynamics. To image the underlying excited state dynamics, we have developed a new spectroscopic method allowing us to probe excitonic dynamics within photosynthetic antenna complexes. New data on the role of the protein in photosynthetic systems indicates that the chromophores mix strongly with some bath modes within the system. The implications of this mixing for excitonic transport will be discussed along with new results showing long-lived coherence in synthetic systems that demonstrate the same underlying design principles.

Greg Engel is an Associate Professor at The University of Chicago in the Department of Chemistry and The James Franck Institute. His research focuses on new approaches to observe, measure, and control excited state reactivity. His group specifically focuses on excitonic transport, open quantum dynamics, and photochemical reaction dynamics. Engel received his A.B. from Princeton University in 1999 and his Ph.D. from Harvard University in 2004. His doctoral work with Prof. James Anderson focused on new techniques for in situ measurement of atmospheric tracers. Engel then moved to UC Berkeley as a Miller Postdoctoral Fellow studying photosynthetic energy transport working with Prof. Graham Fleming. Engel *is currently a member of the executive committee of the ACS Biophysics subdivision and the APS Division of Laser science. Engel has been recognized as a Coblentz Award Winner, Sloane Fellow, Searle Scholar, a PECASE recipient, DARPA Young Faculty Award recipient, AFOSR Young Investigator, DTRA Young Investigator, Dreyfus New Faculty Award recipient, and one of Scientific American's "2007 SciAm50" top fifty leaders in research.*

Professor Sandu **Popescu**, University of Bristol, UK
What is quantum in quantum biology?

In my talk I will describe different types of potential quantum effects in biology and I will discuss their significance. I will also address the issue of entanglement versus simple quantum coherence.

Short Talks

Dr Ahsan **Nazir**, Department of Physics, Imperial College London, UK

Strong coupling master equations for excitonic energy transfer dynamics

Recent experiments demonstrating signatures of quantum coherence in the energy transfer dynamics of a variety of light-harvesting systems have sparked renewed interest in the theoretical modelling of energy transfer processes. A major challenge remains the development of techniques which allow one to probe the diverse parameter regimes relevant to such systems. Master equation methods provide useful tools with which to efficiently analyze energy transfer dynamics in the presence of an external environment. However, they are often valid only in rather restrictive parameter regimes, limiting their applicability in the present context.

Here, I shall present a versatile variational master equation approach to the dynamics of excitation energy transfer, that allows for the exploration of a wide range of parameter regimes within a single formalism [1]. Derived through the combination of a variationally-optimised unitary transformation and the time-local projection operator technique, the formalism can be applied to a range of bath spectral densities, and accounts for both non-Markovian and non-equilibrium environmental effects. Furthermore, I shall show that while it correctly reproduces Redfield, polaron, and Foerster dynamics in the appropriate limits, it can also be used in intermediate regimes where none of these theories may be applicable. I shall also discuss the extension of the theory to many-site energy transfer systems. Variational master equations thus represent a promising avenue for the exploration of energy transfer dynamics in a variety of physical systems.

[1] D. P. S. McCutcheon and A. Nazir, J. Chem. Phys. 135, 114501 (2011); D. P. S. McCutcheon, et al., Phys. Rev. B 84, 081305(R) (2011)

Dr Karoline **Wiesner**, School of Mathematics, University of Bristol, UK

Studying biology with quantum Occam's razor

Given a data sequence such as a time series of a complex system -- a light-harvesting complex, a DNA junction, or a collection of neurons -- we have no method for determining whether quantum mechanical effects are influencing the dynamics on a macroscopic scale without making assumptions on the underlying physical process. In the spirit of Occam's razor, simpler is better; should two models make identical predictions, the one that requires less input is preferred. In recent work we have used quantum mechanics to sharpen Occam's razor as applied to minimal statistical predictors (1). It allowed us to systematically construct quantum models which have smaller entropy than classical models. This indicates that the system of minimal entropy that exhibits such statistics must necessarily feature quantum dynamics, and that certain phenomena could be significantly simpler than classically possible should quantum effects be involved. We will illustrate the formalism with the example of a classical statistical predictor for a DNA junction dynamic [2]. We will discuss experimentally testable criteria for quantum effects and comment on the current investigation into applications to magnetoreception.

[1] M. Gu, K. Wiesner, E. Rieper, and V. Vedral, "Quantum mechanics can reduce the complexity of classical models," Nature Communications, vol. 3, p. 762, Mar. 2012. arxiv/1102.1994
[2] D. Kelly, M. Dillingham, A. Hudson, and K. Wiesner, "A New Method for Inferring Hidden Markov Models from Noisy Time Sequences," PLoS ONE, vol. 7, no. 1, p. e29703, Jan. 2012. arxiv/1011.2969

Dr Janet **Anders**, Department of Physics and Astronomy University College London and
Ms Sania **Jevtic**, Imperial College, UK
Contribution of quantum tunnelling events in chemical rates

Chemical reactions are thought to happen when a particle crosses an energetic barrier and into an energetically favourable state. We compare, for a specific solvable energetic potential, the classical transition state theory (TST) rate with the rate that fully includes quantum effects. Traditional TST is used to estimate the rate that results from classical hopping. The model assumes that an initially equilibrated system is suddenly exposed to a non-equilibrium situation which then results in dynamics an the famous TST reaction rate. Our model traces the same assumptions and extends TST by accounting not only for hopping over the barrier but also the tunnelling through the barrier. In our talk we will discuss the temperature dependence of both rate contributions, predict the qualitative behaviour of the kinetic isotope effect (KIEs) for this particular model and hypothesise what these results imply for reactions catalysed by enzymes.

Dr Sam **Hay**, Manchester Institute of Biotechnology (MIB), University of Manchester, UK
Quantum selection of enzyme substrates?

DNA polymerase, the enzyme family that catalyses DNA replication, has been the object of study for about 50 years, yet the fundamental mechanism these enzymes use to select the correct dNTP substrate from a cellular pool of structurally very similar molecules remains unresolved. During DNA replication, DNA polymerase catalyses the incorporation of the four structurally similar dNTPs into a growing complementary strand of DNA. DNA polymerase appears to follow an ordered binding of substrates, first binding DNA, followed by a dNTP. Upon dNTP binding, a complex set of structural rearrangements in the enzyme are thought to occur, beginning with an 'induced fit'. Clearly, the dNTPs are all quite similar, and if the enzyme cannot pre-select the correct dNTP then at least 3 out of 4 reactions will be aborted. However, if quantum mechanics plays a significant role in dNTP binding then some degree of pre-selection of the correct dNTP may occur if two or more dNTPs became entangled and simultaneously superimposed within the active site of the enzyme. DNA polymerase could then collapse the wavefunction of the enzyme with the correctly bound dNTP. If these proposed quantum dNTP binding events are described by Grover's quantum search algorithm then it would be possible to sample up to four different unsorted states (i.e. dNTP binding events) in a single search (where the "yes/no" query is e.g.: "is the correct dNTP bound"). The possibility of a quantum search of dNTP binding to DNA polymerase was suggested by Patel 10 years. Since then, it has been suggested that DNA annealing may also be influenced by quantum mechanics. We are not aware, however, of any attempt to investigate the role of quantum mechanics during DNA replication – which is more physiologically relevant. We are working towards this using a combination of experimental enzymology and theoretical/computational chemistry.

Dr Martin **Robert**, Keio University, Institute for Advanced Biosciences, Japan

Is the apparent emergent spacio-temporal and multi-scale organization of living systems connected to quantum coherence?

Quantum phenomena are often associated with unfamiliar and poorly understood phenomena that characterize the microscopic world of subatomic particles and other fundamental levels of matter. Quantum theory, as one of the most successful scientific theories may have many implications beyond the microscopic level but these are only beginning to gain attention from the physics community. The possibility of biological systems operating in a quantum coherent way is both attractive and controversial. Traditional models seem to preclude quantum coherence in the warm environments in which most living organisms operate. I would like to suggest that whole cells and even cell population may display basic properties reminiscent of quantum phenomena, including quantum coherence. Support for this idea already seems abundant in biological oscillatory systems, including whole cells. Populations of synchronized cells can display wave-like properties and may undergo interactions simi lar to quantum interference, one of the hallmarks of quantum behavior. Manipulations of such cellular systems can induce or destroy these properties in a process analogous to the quantum to classical transition associated with observation and decoherence. The maintenance of quantum coherence in cells may be made possible by the insulating yet open architecture of the cell membrane and the role of metabolism as a critical mechanism acting against decoherence. In addition, the constant and essential information exchange between elements at all scales of biological organization is a quintessential mechanism for the maintenance of temporal organization and coherence. While the issue of quantum coherence of whole cells or organisms may currently remain unsettled, it may be important to consider a more encompassing view of quantum coherence in living systems. This may lead to novel insights about their unique nature and properties.

Dr Libby **Heaney**, Centre of Quantum Technologies, National University of Singapore

Quantum coherent contributions to electron transport in respiratory complex I

Many intramolecular electron transfer (ET) reactions in biology are mediated by metal centres in proteins. This process is commonly described by a model of diffusive hopping, according to the semiclassical theories of Marcus and Hopfield. However, recent studies have raised the possibility that non-trivial quantum mechanical effects play a functioning role in certain biomolecular processes. Here we investigate the potential effects of quantum coherence in biological ET by extending the semiclassical model to allow for the possibility of quantum coherent phenomena using a quantum master equation based on the Holstein Hamiltonian. We test our model on the structurally-defined chain of seven iron-suphur (FeS) clusters in NADH:ubiquinone oxidoreductase (complex I), a crucialrespiratory enzyme and one of the longest chains of metal centres in biology. Using experimental parameters where possible we find that, in limited circumstances, a small quantum mechanical contribution can provide a marked increase in the ET rate above the semi-classical diffusive-hopping rate. Under typical biological conditions our model reduces to well-known diffusive behavior. We discuss the likelihood of quantum coherent ET in biology and note that our model is general enough to be applied to electron transport elsewhere in biology.

Professor Iannis **Kominis**, University of Crete, Greece

Quantum dynamics of the chemical compass

I will review the quantum dynamics of the chemical compass, a topic which has attracted quite some attention recently. I will explain the intricate dynamics of quantum coherence in the spin-dependent biochemical reactions underlying the chemical compass and resolve current discrepancies and conflicting theoretical descriptions of this system. The relevant papers that I will discuss are the following.

[1] Magnetic Sensitivity and Entanglement Dynamics of the Chemical Compass, I. K. Kominis, arxiv:1111.3974
[2] The Quantum Zeno Effect Immunizes the Avian Compass Against the Deleterious Effects of Exchange and Dipolar Interactions, A. T. Dellis and I. K. Kominis, Biosystems 107, 153 (2012).
[3] Radical-ion-pair reactions are the biochemical equivalent of the optical double slit experiment, I. K. Kominis, Phys. Rev. E 83, 056118 (2011).
[4] Comment on "Spin-selective reactions of radical pairs act as quantum measurements", I. K. Kominis, Chem. Phys. Lett. 508, 182 (2011).
[5] Quantum Zeno effect explains magnetic-sensitive radical-ion-pair reactions, I. K. Kominis, Phys. Rev. E 80, 056115 (2009).

Posters

Dr Agata **Checinska**, Center for Quantum Technologies, National University of Singapore

Energy transfer in donor-acceptor pair: variational transformation approach

We investigate the energy transfer in the donor-acceptor pair interacting with local and global baths. We use variational transformation and time-convolutionless method to derive the corresponding master equation. We look at the situation where spatial correlations between two sites can be present and investigate the interplay between the coherent and incoherent energy transfer. The model can applied to many biological donor-acceptor systems.

Mr Adam **Godbeer**, Professor Jim Al-Khalili and Professor Paul Stevenson, Department of Physics, University of Surrey, UK

Modelling effects of environment on proton tunnelling in asymmetric double-well

The temporal evolution and decoherence of a quantum state in an asymmetric double well potential is investigated using a time-dependent density matrix in the eigenstate basis. The Liouville-von Neumann master equation for open quantum systems [1] is solved for a proton in such a well, in order to model hydrogen bonds between DNA base pairs.

Decoherence is achieved by coupling the potential to a heat bath ("environment"). This is implemented with the addition of a Lindblad term, where transition probabilities are calculated using the methods described by Meyer & Ernst [2] in order to discover whether such coupling to the environment influences tunnelling times. The preliminary results presented here show an oscillatory effect without environment interaction, as expected, taking place on picosecond timescales (depending on the starting conditions).

[1] C. Scheurer and P. Saalfrank, J. Chem. Phys. 104 (1996) 2869

[2] R. Meyer and R. R. Ernst, J. Chem. Phys. 93 (1990) 5518

Dr Stephen **Clark**, Atomic and Laser Physics, University of Oxford, UK

Dephasing enhanced transport in non-equilibrium strongly-correlated quantum systems

Quantum systems can be characterised by a triad of properties: geometry, disorder, and interactions. With this in mind their has recently been intense interest in the counter-intuitive beneficial role that noise can play in improving the efficiency of quantum transport, challenging the conventional notion that external couplings unconditionally degrade performance. In particular the delicate interplay of coherent transport and dephasing processes has been shown to be responsible for the highly efficient excitation transfer in photosynthetic complexes. However, to date the enhancements found are based on disrupting single-particle interference effects arising from only the first two of the triad of properties, namely geometry and disorder. In this work we complete the triad by reporting dephasing enhanced transport in a system that results exclusively from the presence of strong many-body interactions. Using large scale matrix product simulations of the quantum master equation we demonstrate this effect numerically in the non-equilibrium stationary state of a boundary driven XXZ spin chain. We then construct a simple model of this system which highlights how the dominant effect of dephasing is to break-up coherences within an insulating dark-state. This then causes population transfer to a propagating band of excitations and dramatically increases the spin-current. This dephasing enhanced transport is found to only in the strongly interacting regime. Moreover the existence of an enhancement is seen to form an "order parameter" for the non-equilibrium phase transition expected between the weak and strongly interacting limits of this system. Since these effects are based on rather generic features of many-body eigenstates they are conjectured to occur in other interacting systems such as the Hubbard model relevant in describing electron motion in numerous realistic systems.

Mr Juan Jose **Mendoza Arenas**, University of Oxford, UK
Environment-assisted transport in strongly-interacting incoherently-coupled quantum spin chains

Recent experimental observations of long-lived quantum coherences in light-harvesting complexes have triggered an intense research on their effects on energy transfer processes, which during a long time were thought to be of classical nature. This has led to propose that to achieve large transfer efficiencies, a proper balance between coherent and incoherent phenomena is required. In particular, in a conjugated polymeric system (MEH-PPV), intrachain coherent transport has been observed, while interchain hopping has been identified as an incoherent process. In the present work, we study the interplay between coherent intrachain and incoherent interchain transport processes in a simple model, consisting on several strongly-correlated XXZ spin chains incoherently coupled to each other; the planar couplings represent coherent hopping of spins, and the coupling in z direction corresponds to a interaction between excitations. Using the Time Evolving Block Decimation (TEBD) method, we calculate the steady state of the system when it is driven to a non-equilibrium configuration by pumping excitations at the edges of each chain. We observe that below a critical interaction in z direction, the spin current through the system diminishes as the incoherent coupling increases, but above this critical coupling, the current can be strongly enhanced due to incoherent coupling (close to 100% at weak driving, up to several orders of magnitude for strong driving, where a purely coherent evolution turns the system into an insulator). This corresponds to a new mechanism of environmentassisted transport, which in contrast to previously reported ones, is a genuine many body phenomena. We discuss the nature of this mechanism, which is based on the breaking of bound spin states, initially formed due to their strong interaction, by incoherent effects. We expect this effect to be very important for light-harvesting systems, where strong interactions between exci tations might arise.

Mr Vahid **Salari**, IMPMC, UPMC, Paris, France
Nano-bio-refrigerators in excitable cells

The selectivity filter (SF) of ion channel proteins (ICP) is responsible for the selective and fast conduction of ions across the membrane of an excitable cell. After the determination of an atomic resolution structure of the bacterial KcsA channel by Mac Kinnon (the winner of 2003 Nobel prize in chemistry), the question was raised whether the SF can also adopt non-conducting states, acting as a ‘filter-gate’ and how these states could become synchronized with the mechanical opening and closing of the pore-domain gate facilitating conduction. The ‘selectivity’ can be attributed to the specific Coulomb-coordination geometry between the ion and the surrounding dipolar carbonyl ligands lining the so-called P-loop domain of the filter region. Recently, some efforts have been done to find the quantum effects inside the SF structure theoretically and experimentally. Here, based on our MD simulations and investigation of the all possible frequencies of carbonyl groups of SF (for thermal and transmembrane potential energies via Gaussian software) we have found a strong ‘cooling’ effect of ions inside the SF which can have important effects on neural communication and signal transfer. In conclusion, we show that SF acts like a strong nano-bio-refrigerator.

“A Parable of a Physicist and Twin Torsos” - Painting
Mr Carl **Gopalkrishnan**, Visual Artist, Western Australia and Professor Caslav **Brukner**, Faculty of Physics, University of Vienna

Caslav and I have shared correspondences about quantum physics and art since 2006 when I first started making the link with the quantum world and our human gaze. This painting, *The Parable of the Physicist*, is part of a new series which explores the spiritual dimension of our post-human consciousness. How will engineered life come to pass, and how might quantum entanglement influence this *immaculate* conception?

The germ of this series began with a storyline around solar storms and actual replica torsos used by both NASA and European Space Agency called *Fred and Matryoshka* that reminded me of *Romulus and Remus* the mythical founders of ancient Rome, used to investigate the effect of this radiation on astronauts. This opened up other questions for me like how these eruptions might affect our DNA and if the way we conceive of ‘human’, ‘non-human’ and ‘machine’ is all linked at the quantum level. So, that’s how The Twins came about and Caslav became those Twins in my painting. The DNA question continued in reference to the gene synthesis company Blue Heron, that also appear as actual birds.

The rest emerged from my dreams - especially the two red nuclear submarines (Typhoon Class). When I completed it, I noticed there were 2 of everything, like two entangled particles. A lot came out through the back door (my subconscious). And in that sense, I really did channel the Surrealists in the way that the pictorial elements emerged. But the 'two-of-everything' also reminded me of *Noah's Ark*, and thus my biblical reference to a parable, where the physicist is performing an unusually spiritual function, so the whole idea of biology and entanglement together gave the painting this feeling of a parable. And in the context of a new series of paintings, this is a "thought-in-progress".

Caslav is very generous and inspiring and understood about the lens, because the act of looking (the gaze) is integral to both entanglement theory and to this painting. [Carl Gopalkrishnan, Australia, 2012]

"In classical physics and everyday life every object has well-defined properties on its own. Every dice has its well defined faces, and every person has its own individuality. According to quantum theory, however, two or more entangled objects can have perfectly defined joint properties at the expense of losing their individual properties. This is like having two persons with no individual properties, no phenotype, no character, until they are subject to observation, upon which they obtain a random but same face, same character, same gender, i.e. they become identical twins. Likewise two entangled dices have no orientation on their own until they are measured, upon which they show the same random side up." [Caslav Brukner, Vienna, 2012]

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