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ABSTRACTS OF POSTERS

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Motional effects on the efficiency of excitation transfer in photosynthetic complexes

Ali Asadian [Innsbruck University]

Motion and conformational changes are ubiquitous features in biological systems. Moreover, it is well-known that biological systems exploit their dynamical behaviour to better perform their tasks. In this work we study the effects of oscillatory molecular motion on excitation transfer. We investigate two normal modes of spatial oscillation, namely the breathing and slashing mode, in which each bio-unit oscillates with the same frequency. Our numerical simulations demonstrate that oscillations in a suitable range of frequencies can significantly enhance the efficiency of energy transfer. This enhancement has no classical analog in Förster theory and seems to derive from the collaboration between coherent excitation transfer and overimposed classical molecular motion.

Joint work with Jianming Cai, Gian Giacomo Guerreschi, and Hans Briegel [Innsbruck University].

Quantum entanglement and off-equilibrium thermodynamics of oscillating molecules

Jianming Cai and Gian Giacomo Guerreschi [Innsbruck University]

We demonstrate that entanglement can persistently recur in an oscillating two-spin molecule that is coupled to a hot and noisy environment, in which no static entanglement can survive. The system represents a non-equilibrium quantum system which, driven through the oscillatory motion, is prevented from reaching its (separable) thermal equilibrium state. Environmental noise, together with the driven motion, plays a constructive role by periodically resetting the system, even though it will destroy entanglement as usual. As a building block, the present simple mechanism supports the perspective that entanglement can exist also in systems which are exposed to a hot environment and to high levels of de-coherence, which we expect e.g. for biological systems. Our results furthermore suggest that entanglement plays a role in the heat exchange between molecular machines and environment. Experimental simulation of our model with trapped ions is within reach of the current state-of-the-art quantum technologies.

Joint work with Hans Briegel [University of Innsbruck].

Quantum entanglement in photosynthetic processes

Animesh Datta [Imperial College]

We show for the first time, albeit theoretically, the explicit presence of quantum entanglement (as quantified by the negativity) in a naturally occurring photosynthetic system. We will discuss the functional role of entanglement in the process of photosynthesis. We will present evidence that environmental noise processes that tend to enhance transport actually suppress the amount of entanglement. This might lead us to believe that entanglement is a byproduct of the coherent part of the evolution, rather than playing a nontrivial role in driving the process.

Joint work with Alex. W. Chin, Filippo Caruso, Susana F. Huelga, and Martin B. Plenio [University of Hertfordshire and Imperial College].

Wave-particle duality of large molecules revealed

Thomas Juffmann [University of Vienna]

Molecular interferometry has proven to be a suitable tool for testing the wave-particle duality of large, heavy and hot molecules [1], some of which are also relevant in biological systems [3]. However, experiments on thermal [2] and collisional [4] decoherence also showed the fragility of these quantum properties. Here, we report on a new detection scheme for molecular interferometry: the near-_eld interference pattern is deposited onto a detection surface, which is subsequently imaged using various microscopic techniques. Scanning tunneling microscopy even allows to image every single molecule with nanometer resolution within the interference pattern, revealing the wave-particle duality in its clearest form. First interferograms of C60 molecules deposited onto reconstructed Si(111)7x7 are presented. This method is not only intuitive and most sensitive, but also intrinsically scalable to larger biomolecules or clusters. Alternative detection schemes using AFM or uorescence microscopy will be discussed.

References: [1] M. Arndt, O. Nairz, J. Voss-Andreae, C. Keller, G. Van der Zouw, and A. Zeilinger. Waveparticle duality of C60 molecules. Nature, 401:680, 1999. [2] L. Hackermuller, K. Hornberger, B. Brezger, A. Zeilinger, and M. Arndt. Decoherence of matter waves by thermal emission of radiation. Nature, 427:711, 2004. [3] L. Hackermuller, S. Uttenthaler, K. Hornberger, E. Reiger, B. Brezger, A. Zeilinger, and M. Arndt. Wave nature of biomolecules and uorofullerenes. Phys. Rev. Lett., 91:90408, 2003. [4] K Hornberger, S Uttenthaler, B Brezger, L Hackermuller, M Arndt, and A Zeilinger. Collisional decoherence observed in matter wave interferometry. Phys. Rev. Lett., 90(16), APR 25 2003.

Joint work with Stefan Truppe, Philipp Geyer, Michael Mullneritsch, Sarayut Deachapunya, Andras Major, Hendrik Ulbricht, and Markus Arndt [University of Vienna].

Spectral modulation of carotenoids by the protein environment

Mindaugas Macernis [Vilnius University]

The regulation of photosynthetic light harvesting is a physiologically significant strategy evolved by plants. Rapid excitation density control in photosystem II (PSII), termed as non-photochemical quenching (NPQ), ensures efficient functioning of the plant photosynthesis under very different light conditions up to very high intensities. To make any conclusive decisions concerning their possible role in NPQ the lowest excited states of carotenoids and their sensitivity to the protein environment should be well conceived. Here we present our studies of the excited states of carotenoids (lutein and zeaxanthin) using quantum chemical calculations. Doubly excited configurations are essential in order to achieve first excited singlet state (it is dark state for all planar states of lutein and zeaxanthin). The account of the influence of double excited configurations was reached by using Tamm-Dancoff approximation density functional theory method (TDa-DFT/blyp) [1]. CI SD, CI SDTQ and MCSCF PT2 methods were used for testing computations for different lutein conformations known from the crystallographic data of LHCII complexes. Lutein conformation and spectra are highly dependant on the surrounding environment. The influences of deformation of polyene chain and aromatic rings on the energy positioning and the oscillator strengths of the optical transitions of the S1 and S2 states depending on the surrounding environment have been investigated by means of TDa-DFT/blyp and QM/MM methods. Reference: Dreuw, J. Phys. Chem. A, 110, 4592-4599 (2006).

Joint work with Juozas Sulskus and Leonas Valkunas [Vilnius University].

Decoherence assisted excitonic energy transfer

Alejandro Perdomo [Harvard University]

Coherence can play a significant role in the efficiency of excitonic energy transfer. Realistic scenarios for antenna subunits in artificial solar cell candidates are unavoidably exposed to decoherence effects due to additional degrees of freedom which cannot be included explicitly in the dynamics of the system. In this work, we present strategies to cope with decoherence effects and to use decoherence to enhanced energy transfer to a particular site. Examples of directed excitonic motion in quantum dots are shown, where by engineering the environment and energy levels, one can guide the motion of the excitation to places which will not be favored by a fully quantum coherent picture. We will also discuss the possibility of using electronic structure methods to obtain the relevant parameters that determine this decoherence enhanced mechanism in the case of molecular systems.

Joint work with Ali Najmaie, Leslie Vogt, and Alan Aspuru-Guzik [Harvard University].

Noise and entanglement of current flowing through dissipative quantum dot chains

Katarzyna Roszak [Charles University and Wrocław University of Technology]

The enhancement of electron transport efficiency through chains of two level systems due to decoherence has inspired a lot of interest recently. This is both because of the counter-intuitive feature of dephasing-assisted phenomena [1] as well as the possible importance of such processes in biological systems [2]. Among other things, the study of the current (shot) noise is an efficient tool for distinguishing between various quantum and classical features in stationary electronic transport [3]. It may be therefore useful also for the study of two-level system (exciton) chains and may serve to bring a better understanding of the underlying physical mechanisms. We study the noise properties of electrical current through short quantum dot chains under the influence of a phonon-induced dephasing channel. An analogous phenomenon to the dephasing/dissipation-enhanced transport has been recently observed experimentally [4] and understood theoretically [4, 5, 6] in semiconducting double quantum dots. We modify the established setup by considering instead the energy transport via molecular excitons with qualitatively similar results. We correlate the shot noise behaviour with the entanglement measures [7, 8, 9] and point out surprising connection between the “quantumness” of the exciton hopping underlying process and character of the memory in the corresponding non-Markovian master equation [6]. Furthermore, we draw attention to technical issues related to a consistent theoretical description of the systems exhibiting interplay between coherence and dissipation within the generalized master equation approaches [10]. Our results can be ext ended from double quantum dots to longer chains. References: [1] M. B. Plenio and S. F. Huelga, New Journal of Physics 10, 113019 (2008). [2] G. S. Engel et al., Nature 446, 782 (2007). [3] Y. Blanter and M. Buttiker, Phys. Rep. 336, 1-166 (2000). [4] G. Kießlich et al., Phys. Rev. Lett. 99, 206602 (2007). [5] R. Sánchez et al., Phys. Rev. B 77, 035409 (2008). [6] A. Braggio, C. Flindt, and T. Novotný, Physica E 40, 1745 (2008). [7] N. Lambert, R. Aguado, and T. Brandes, Phys. Rev. B 75, 045340 (2007). [8] C. W. J. Beenakker et al., Phys. Rev. Lett. 91, 147901 (2003). [9] P. Samuelsson, E. V. Sukhorukov, and M. Büttiker, Phys. Rev. Lett. 91, 157002 (2003). [10] J. Prachař and T. Novotný, arXiv:0902.2382 (2009).

Joint work with Tomáš Novotný [Charles University].