WORKSHOP PROGRAM

http://fama.iff.csic.es/fama/con/MWOQS-2011/
Welcome to the Madrid Workshop on Open Quantum Systems, MWOQS-2011!

The goal of this workshop is to bring together young and more advanced researchers currently involved in the study of system-environment interactions.

Over the past few years there has been intense interest in the study of systems interacting with their environment, from regimes where the latter is characterized by fast fluctuations (Markovian models) to other, more complicated situations where the system vs bath time scales are similar. In the latter case, more refined, non-Markovian models have to be developed.

The meeting is expected to cover a broad range of physical problems where system-environment interactions are relevant, such as quantum transport phenomena, energy transfer processes or quantum information processing, as well as the theoretical and numerical techniques designed in the last years to tackle them.

This is an initiative of the COST Action Fundamental Problems in Quantum Physics (in particular, the working group Effective description of complex systems), aimed at encouraging the formation of a united platform of researchers devoted to the full understanding of quantum processes and phenomena at a fundamental level.

The Organizers

Irene Burghardt
Institut für Physikalische und Theoretische Chemie, Goethe-Universität (Frankfurt, Germany)

Ángel S. Sanz
Instituto de Física Fundamental - CSIC (Madrid, Spain)
## WORKSHOP PROGRAM

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Heavy atom quantum diffraction by scattering from surfaces
Eli Pollak

Quantum Zeno and anti-Zeno effects in surface diffusion of interacting adsorbates
Salvador Miret-Artés

Session 2 (Vacchini): Non-Markovian dynamics and open quantum systems
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Luca Ferialdi

Trace-distance analysis of initial correlations in the dynamics of open quantum systems: Theory an experiment
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Characterizing open quantum systems through information flow
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Session 3 (Bassi): Approaches to non-Markovian Dynamics
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Jyrki Piilo

Markovian and non-Markovian dynamics in quantum and classical systems
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Non-Markovian open systems: Input-output theory
Lajos Diósi
Session 4 (Diósi): Quantum transport phenomena
Excess noise induce transport
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Spin-polarized currents in double and triple quantum dots driven by ac magnetic fields
María Busl

Phonon-mediated decoherence in triple quantum dot interferers
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Session 5 (Piilo): Cold system dynamics and quantum control
Coherent backscattering effect: The case of ultracold matter waves
Nicolas Cherroret

Non-destructive spectroscopy on cold molecular ions
Jesús Pérez-Rios

Quantifying, characterizing and controlling information flow in ultracold atomic gases
Pinja Haikka

Tuesday, October 4

Session 6 (Pollak): Quantum coherence and correlations
Quantum coherence in photosynthetic exciton dynamics
Peter Nalbach

Non-perturbative simulations of exciton dynamics in complex biological environments
Javier Prior

Quantum similarity index: Generalization and applications in multielectronic systems
Juan Carlos Angulo

Session 7 (Miret-Artés): Quantum Trajectories and Bohmian mechanics
Classical-like trajectory simulation of quantum cumulative reaction probabilities
Gerard Parlant

Computing quantum open systems with Bohmian trajectories: The role of the conditional wavefunction
Xavier Oriols
**Session 8 (Hughes): Quantum, classical and semiclassical evolution**
Partial linearized density matrix dynamics for dissipative, non-adiabatic quantum evolution
David Coker

Beating the efficiency of both quantum and classical simulations with semiclassics
Jiri Vanicek

Fractal Weyl law behavior in an open Hamiltonian system
Florentino Borondo

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Phase space master equations for quantum Brownian motion in a periodic potential: Comparison of various kinetic models
William T. Coffey

Quantum correlations and quantum synchronization
Roberta Zambrini

How real are time-local master equations?
Daniel Maldonado Mundo

Green function for the classical and quantum Kramers’ turnover problem
Declan Byrne

**Wednesday, October 5**

**Session 10 (Parlant): Quantum transport and dynamics in nanoscale systems**
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Sigmund Kohler

Coherent dynamics of electrons in ac driven quantum dot arrays
Gloria Platero

Towards decoherence studies in optical microfibers
Manfred Niehus

**Session 11 (Burghardt): Open quantum system dynamics**
Decay and entanglement with reservoir structures
Barry M. Garraway

Hierarchical effective mode approach to non-Markovian reduced dynamics
Keith H. Hughes
ABSTRACTS
Heavy atom quantum diffraction by scattering from surfaces

Jeremy M. Moix and Eli Pollak
Chemical Physics Department, Weizmann Institute of Science, Israel

Typically one expects that when a heavy particle collides with a surface, the scattered angular distribution will follow classical mechanics. The heavy mass usually assures that the coherence length of the incident particle in the direction of the propagation of the particle (the parallel direction) will be much shorter than the characteristic lattice length of the surface, thus leading to a classical description. Recent work on molecular interferometry has shown that extreme collimation of the beam creates a perpendicular coherence length which is sufficiently long so as to observe interference of very heavy species passing through a grating. Here we show, using quantum mechanical simulations, that the same effect will lead to quantum diffraction of heavy particles colliding with a surface provided that the surface temperature is sufficiently low (see the figure below, plotted for the scattering of an Ar atom from a LiF surface). The effect is robust with respect to the incident energy, the angle of incidence and the mass of the particle. Increasing the surface temperature changes the nature of the scattering distribution from a quantum diffraction pattern to a classical rainbow pattern. Collimated heavy particle scattering from surfaces can thus probe the transition from coherent quantum scattering to incoherent classical like scattering.

Quantum Zeno and anti-Zeno effects in surface diffusion of interacting adsorbates

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In this work, two fundamental phenomena of quantum dynamics, namely the quantum Zeno and anti-Zeno effects, are analyzed in the context of surface diffusion of interacting adsorbates. After introducing in a very simple and general fashion the physical implications of both effects within the theory of measurement at two surface temperature regimes (high and very low or even zero), the quantum intermediate scattering function for adsorbate diffusion on flat surfaces is evaluated, which is fully analytical. The generalization to corrugated surfaces is also discussed, finding that, within a Markovian framework and high surface temperatures, the anti-Zeno effect has already been observed, although it has not been recognized as such.
Historically, Markovian quantum time evolutions were associated to the Kossakowki-Lindblad form of master equations and, as a consequence, all of the quantum dynamical equations which could not be recast in the Kossakowski-Lindblad form were called non-Markovian. However, the existence of time-dependent Kossakowski-Lindblad forms has lately attracted the attention of several groups asking for a broad definition of Markovianity and quantifying deviations from it. Actually the very definition of a non-Markovian process has very recently given rise to a vivid debate in the scientific community [1-4].

Here we present a summary of the different concepts non-Markovianity and show a way to unify them. Thus, we propose a unique solution for the problem of how to define Markovianity. This takes the advantage of previous ideas and approaches leading to a well-defined mathematical property which, in addition, enjoys an operational meaning.

Furthermore, we review some of the recently proposed measures of non-Markovianity explaining their meaning and how to compute them.

Stochastic Schrödinger equations and non-Markovian open quantum systems

Luca Ferialdi
Department of Physics, Università di Trieste, Italy

Stochastic Schrödinger equations are a powerful mathematical formalism which give deep insight into physical systems, like e.g. collapse models. We show that open quantum systems allow for a stochastic unravelling, where the environment is described by a noise. Moreover, this approach allows for analytic treatment of non-Markovian open quantum systems, which are described by a noise with a general time correlation function.
Trace-distance analysis of initial correlations in the dynamics of open quantum systems: Theory and experiment

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The dynamics of an open quantum system interacting with an environment is usually described by means of completely positive trace preserving maps on the state space of the open system. The very existence of such maps generally requires that the initial correlations between the open system and the environment can be neglected. However, this assumption is not always physically justified, especially outside the weak coupling regime. Thus, it becomes of interest to introduce different strategies in order to characterize the open-system dynamics in the presence of initial system-environment correlations.

An approach for the study of initial correlations that is based on the use of the trace distance has been introduced in [1]. The trace distance between two states of an open quantum system quantifies their distinguishability, and, for a fixed environmental state, can increase above its initial value only in the presence of initial correlations. In the first part of my contribution, the general theoretical scheme as well as its first experimental realization [2] are presented. The latter has been performed by the quantum optics group at the University of Milan through an all-optical apparatus, in which spontaneous parametric down conversion is exploited as a source of polarization entangled states, and a spatial light modulator introduces in a general fashion correlations between the polarization and the momentum degrees of freedom, which act as environment.

After that, the paradigmatic and exactly solvable model provided by the Jaynes-Cummings Hamiltonian is briefly discussed [3]. In particular, the correlations contained in the thermal equilibrium state for the total system are considered, showing their connection to the entanglement properties of the eigenstates of the Hamiltonian. The trace-distance evolution of the open system states evolving from the thermal state and its corresponding uncorrelated product state shows that the open system dynamically uncovers typical features of the initial correlations.

Characterizing open quantum systems through information flow

Elsi-Mari Laine\textsuperscript{a}, Heinz-Peter Breuer\textsuperscript{b} and Jyrki Piilo\textsuperscript{a}

\textsuperscript{a}Turku Center for Quantum Physics, Department of Physics and Astronomy, University of Turku, Finland
\textsuperscript{b}Physikalisches Institut, Universität Freiburg, Freiburg, Germany

We study different characteristics of open quantum systems from the perspective of information flow between the open quantum system and the environment. The information flow between the open system and the environment can be seen as a change in the distinguishability between the open system states. This formalism allows us to characterize many features of open quantum systems without referring to any specific representation of the dynamics.

Especially we study the evolution of a general open quantum system when the system and its environment are initially correlated. We show that the trace distance between two states of the open system can increase above its initial value, and derive tight upper bounds for the growth of the distinguishability of open system states. This represents a generalization of the contraction property of quantum dynamical maps. The obtained inequalities can be interpreted in terms of the exchange of information between the system and the environment, and lead to a witness for system-environment correlations which can be determined through measurements on the open system alone. We introduce a measurement scheme to detect initial correlations, which neither requires a knowledge of the structure of the environment or of the system-environment interaction, nor a full knowledge of the initial system-environment state.

Experimental control of the transition from Markovian to non-Markovian dynamics of open quantum systems

B.-H. Liu\textsuperscript{a}, L. Li\textsuperscript{a}, Y.-F. Huang\textsuperscript{a}, C.-F. Li\textsuperscript{a}, G.-C. Guo\textsuperscript{a}, E.-M. Laine\textsuperscript{c}, H.-P. Breuer\textsuperscript{b} and J. Piilo\textsuperscript{c}

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Realistic quantum mechanical systems are always exposed to an external environment. The presence of the environment often gives rise to a Markovian process in which the system loses information to its surroundings. However, many quantum systems exhibit a pronounced non-Markovian behavior in which there is a flow of information from the environment back to the system, signifying the presence of quantum memory effects [1]. The environment is usually composed of a large number of degrees of freedom which are difficult to control, but some sophisticated schemes for modifying the environment have been developed. The physical realization and control of dynamical processes in open quantum systems plays a decisive role, for example, in recent proposals for the generation of entangled states for schemes of dissipative quantum computation, for the design of quantum memories and for the enhancement of the efficiency in quantum metrology. We report an experiment which allows through selective preparation of the initial environmental states to drive the open system from the Markovian to the non-Markovian regime, to control the information flow between the system and the environment, and to determine the degree of non-Markovianity by direct measurements on the open system [2].

\begin{itemize}
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Markovian and non-Markovian dynamics in quantum and classical systems


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c Physikalisches Institut, Universitaet Freiburg, Hermann-Herder-Strasse 3, D-79104 Freiburg, Germany

We discuss the conceptually different definitions used for the non-Markovianity of classical and quantum processes. The well-established definition for non-Markovianity of a classical stochastic process represents a condition on the Kolmogorov hierarchy of the n-point joint probability distributions. Since this definition cannot be transferred to the quantum regime, quantum non-Markovianity has recently been defined and quantified in terms of the underlying quantum dynamical map, using either its divisibility properties or the behavior of the trace distance between pairs of initial states. Here, we investigate and compare these definitions and their relations to the classical notion of non-Markovianity by employing a large class of non-Markovian processes, known as semi-Markov processes, which admit a natural extension to the quantum case. A number of specific physical examples is constructed which allow to study the basic features of the classical and the quantum definitions and to evaluate explicitly the measures for quantum non-Markovianity. Our results clearly demonstrate several fundamental distinctions between the classical and the quantum notion of non-Markovianity, as well as between the various quantum measures for non-Markovianity.

Non-Markovian open systems: Input-output theory

L. Diósi

Research Institute for Particle and Nuclear Physics, Budapest, Hungary

The input-output field theory of Gardiner and Collet [1] is applied to non-Markovian open quantum systems for the separation of the memory and detector parts, respectively, of the environmental bath [2]. The system-plus-memory is claimed to be Markovian, the detector part is tractable by standard Markovian monitoring. The corresponding non-Markovian stochastic Schrödinger equation turns out to be the equation [3] from 19, this time in more transparent variables from the viewpoint of the memory structure. Because of non-Markovianity, only the mixed state of the system can be predicted, the pure state of the system can be retrodicted.

Excess noise induced transport

Rafael Sánchez\textsuperscript{a} and Markus Büttiker\textsuperscript{b}

\textsuperscript{a}Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain
\textsuperscript{b}Département de Physique Théorique, Université de Genève, Switzerland

To demonstrate that the relative stability of non-equilibrium states cannot be found from local criteria, Landauer showed that hot spots in locations of phase space that might be only rarely visited can be decisive. Later, Büttiker [1] and van Kampen [2], investigated the noise induced transport generated by hot spots in systems with overdamped Brownian motion dynamics.

In electrical circuits hot spots occur naturally at places where energy is dissipated. Here we propose a controlled experiment which can demonstrate the appearance of directed current as a consequence of a hot spot. We investigate transport generated in Coulomb coupled electrical conductors from excess electric or thermal fluctuations at the coupling capacitance. Gate effects will be emphasized.

If one of the conductors supports a bias voltage, out of equilibrium charge fluctuations remove detailed balance in the unbiased system manifested in a drag current. Nonlinear fluctuation relations can nevertheless be obtained [3].

Coulomb coupled conductors permit separate directions of the heat and current flux [4]. In our model, one of the conductors is connected via only one lead to a hot reservoir. The other conductor connects to two leads. We investigate the minimal conditions needed to generate directed current flow for a system of two quantum dot conductors in which both energy and charge states are quantized. In quantum dots energy to current conversion can be optimal with one electron transferred for every heat quantum given up by the hot reservoir. We show that at the point of maximum power extraction the efficiency approaches one half of the Carnot efficiency.

Spin-polarized currents in double and triple quantum dots
driven by ac magnetic fields

Maria Busl and Gloria Platero
Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain

We analyze transport through both a double quantum dot and a triple quantum dot with inhomogeneous Zeeman splittings in the presence of crossed dc and ac magnetic fields. We find that strongly spin-polarized current can be achieved by tuning the relative energies of the Zeeman-split levels of the dots, by means of electric gate voltages: depending on the energy-level detuning, the double quantum dot works either as spin-up or spin-down filter. We show that a triple quantum dot in series under crossed dc and ac magnetic fields can act not only as spin filter but also as spin inverter.

Phonon-mediated decoherence in triple quantum dot interferometers

Fernando Domínguez, Sigmund Kohler and Gloria Platero
Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Spain

We investigate the influence of decoherence on the electronic transport through a triple quantum dot in a ring configuration. In the absence of decoherence and for a certain symmetry, single electron transport gets blocked because an electron falls into a pure state that is decoupled from the electron reservoirs. It is known as dark state. Decoherence enters by the coupling of the system to a damped phonon mode, which destroys the dark state and thus restores a finite current.

We study [1] the current and its shot noise numerically with a generalized master equation approach for the electrons and the dissipative phonon mode. Moreover, we derive an effective master equation for only the electrons by performing a polaron transformation and tracing out the phonon degree of freedom. By means of this transformation the influence of the interaction with the phonon mode is recast in two terms. One of the terms provides incoherent tunnel rates coming from energy conserving transitions and the other one accounts for decoherence produced by the indirect coupling of the dissipative bath of oscillators coupled to the phonon mode. This approach allows one to interpret the decoherence mechanism observed in the numerical results and also to obtain analytical results that agree rather well with the numerical ones.

Coherent backscattering effect: The case of ultracold matter waves

Nicolas Cherroret

Institute of Physics, Albert-Ludwigs University of Freiburg, Germany

In this talk, I will briefly review recent developments concerning the coherent backscattering (CBS) effect, a well-known precursor of Anderson localization in disordered systems. I will then focus on the particular and important case of CBS of ultracold matter waves in random (optical) potentials, and explain how this effect manifests itself in the momentum distribution of the matter wave. A detailed theoretical analysis of this distribution shows that the CBS effect can be used to prove that transport occurs in the phase-coherent regime, and that measuring its time dependence permits monitoring the transition from classical diffusion to Anderson localization.
Non-destructive spectroscopy on cold molecular ions


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*b* Department of Chemistry, University of Basel, Switzerland

We propose an efficient and accurate scheme to perform spectroscopy of molecular ions by implementing quantum logic between an atomic ion and a molecular ion. Our proposal relies on a hybrid manipulation of the system, using optical forces for the atomic ion and magnetic field gradients on the molecular ions. The gate may operate in times that range from $10 \mu s$ to $1$ ms and it is insensitive to the temperature of the ion crystal. One immediate application is the non-destructive measurement of a molecular hyperfine state, thus improving on recent advances in initializing cold molecular ions in a well-defined quantum state [1].

Quantifying, characterizing and controlling information flow
in ultracold atomic gases

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\textsuperscript{c}Física Teòrica: Informació o Fenòmens Quàntics, Universitat Autònoma de Barcelona, Spain
\textsuperscript{d}Center for Theoretical Atomic, Molecular and Optical Physics, School of Physics, Queen’s University, Belfast, UK
\textsuperscript{e}NEST Instituto Nanoscienze-CNR and Dipartemento di Fisica, Università degli Studi di Palermo, Italy

We study quantum information flow in a model comprising of a trapped impurity qubit immersed in a Bose-Einstein condensed reservoir [1]. We demonstrate how information flux between the qubit and the condensate can be manipulated by engineering the ultracold reservoir within experimentally realistic limits. We show that this system undergoes a transition from Markovian to non-Markovian dynamics, which can be controlled by changing key parameters such as the condensate scattering length. In this way one can realize a quantum simulator of both Markovian and non-Markovian open quantum systems, the latter ones being characterized by a reverse flow of information from the background gas (reservoir) to the impurity (system).

Quantum coherence in photosynthetic exciton dynamics

Peter Nalbach

Institute für Theoretische Physik, Universität Hamburg, Germany

Recent experiments suggest that quantum coherence survives in photosynthetic light-harvesting complexes for up to a picosecond despite strong vibrational and polarization environmental fluctuations. This has led to speculations that the lossless exciton transfer is a result of quantum coherent dynamics. I will present numerically exact results for the electronic energy transfer dynamics in the Fenna-Matthews-Olson (FMO) molecular aggregate. In particular, we determine its single excitation subspace dynamics within an open quantum dynamics approach. Depending on the model used, we find quantum coherent dynamics with coherence times exceeding experimentally observed times but also shorter times and even strongly overdamped decay of the site populations. Thus, theoretical understanding at the present stage can neither support nor rule out a picture of quantum coherent energy transfer in natural photosynthesis.
Non-perturbative simulations of exciton dynamics in complex biological environments

Javier Prior
Departamento de Física Aplicada, Universidad Politécnica de Cartagena, Spain

Multi-component quantum systems in strong interaction with their environment are getting increasing attention due to their importance in the accurate description of charge and energy transfer in bio-molecular aggregates. Unfortunately, these systems are very difficult to simulate as the system-bath interactions cannot be treated perturbatively and standard approaches are not valid or inefficient. Here we combine the Time-Evolving Block Decimation (TEBD) methods with novel techniques from the theory of orthogonal polynomials (OP) to provide an efficient method for simulating open quantum systems, including spin-boson models and their generalizations to multi-component systems. The OP theory will map a Hamiltonian representing a quantum system coupled linearly to a continuum of bosonic or fermionic modes to a Hamiltonian that describes a one-dimensional chain with only nearest neighbor interaction. The transformed system is now amenable for efficient numerical simulation using t-DMRG and matrix product states.
Quantum similarity index: Generalization and applications
in multielectronic systems

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A Generalized Quantum Similarity Index is defined, quantifying the similarity among density functions [1]. The generalization includes, as new features (i) comparison among an arbitrary number of functions, (ii) its ability to modify the relative contribution of different regions within the domain, and (iii) the possibility of assigning different weights to each function according to its relevance on the comparative procedure. The similarity among atomic one-particle densities in both conjugated spaces, and neutral–cation similarity in ionization processes are analyzed. The results are interpreted attending to shell-filling patterns, and also in terms of experimentally accessible quantities of relevance in ionization processes.

The recent explosion in knowledge-based chemical research has created a surge of interest in chemical similarity. Molecular modeling and molecular similarity [2] are simple examples of such an interest. More recently the molecular quantum similarity framework has been used to provide a new set of quantum quantitative structure–properties relationship procedures (QQSPR) [3].

For the case of molecules or atoms this kind of similarity measures have been defined as the scalar product between the first order density functions weighted with a bielectronic definite positive operator. The simplest choice, the Dirac delta operator, leads to the well-known Quantum Similarity Index (QSI) [4]. Recent applications of the QSI to the analysis of atomic structure [5] and the changes suffered by the electronic cloud as a consequence of ionization [6] have been carried out. A relevant conclusion arising from those studies is the essential role played by the density in momentum space, as compared to the position one, in order to get non-trivial information from the atomic QSI values. The generalized QSI provides complementary results from a position-space-based study, which are masked when dealing with the pioneering QSI.

A detailed numerical analysis is presented, from which it is clearly established the relationship between valence subshell properties of the systems under comparison and the generalized similarity values, as well as the detection of the presence of systems suffering from anomalous shell-filling.

Classical-like trajectory simulation of quantum cumulative reaction probabilities

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Based on the de Broglie-Bohm formulation of quantum mechanics [1], quantum trajectories have seen a growing interest in the chemical dynamics community over the past ten years or so [2]. Traditionally, "analytic" quantum trajectories, often used as an interpretative tool, were extracted from conventional wave packets. In the more recent “synthetic” quantum trajectory methods, both the trajectories and the wave function are computed on the fly, each affecting the propagation of the other [2]. In a recent article [3], one of the authors showed that it is possible to develop a mathematical formulation of quantum mechanics based exclusively on real-valued trajectories, thus discarding the reference to the wave function altogether. In this article, a 4th-order Newtonian-like ordinary differential equation (ODE) was derived that describes 1D stationary scattering states exactly, solely in terms of quantum trajectories.

In the present work, the 4th-order Newtonian-like ODE is solved for a 1D Eckart barrier system [3]. The propagation of this ODE by means of an adaptive time stepsize integrator turns out to be remarkably stable and accurate, even when the Eckart barrier exhibits extreme reflection interference.

The remarkable behavior of the above mentioned equation is further exploited in the study of a 2D bottleneck-type problem, a prototype for chemically reactive systems. The quantum Newtonian-like equation is used for the reaction coordinate while the vibrational coordinate is treated classically. Cumulative reaction probabilities (CRPs) are obtained by summing transmission probabilities over trajectories, using a new sampling scheme based on quasiclassical phase space approximations to initialize the classical phase space coordinates. Excellent agreement with exact quantum calculations is obtained over a large energy range, including energies below the reaction barrier threshold where tunneling is large.


Computing quantum open systems with Bohmian trajectories:

The role of the conditional wavefunction

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The fact that a direct solution of the Schrödinger equation is inaccessible for more than 3, 4, 5 degrees of freedom (i.e. the so-called many-body problem) is the reason why any (closed) system has to be “opened” by eliminating many (internal or/and external) degrees of freedom. Unfortunately, such elimination introduces limitations on the predicting capabilities of these approximated solutions. Thus, during the last century, many attempts have been developed in the literature to provide quantum formalisms that are able to deal with a large (but not all) number of degrees of freedom, by avoiding the direct solution of the Schrödinger equation. The quantum Monte Carlo techniques, Hartree-Fock or Density Functional Theory (DFT), among others, are examples of the great success of these formalisms to tackle many-body problems in condensed matter, physical chemistry, nanoelectronics, optics, etc.

In this conference, we present an alternative formalism developed recently in order to approximate the many-body problem within Bohmian mechanics \cite{1,2}. The computational difficulties of solving the many-particle Schrödinger equation arise because the wavefunction \( \Psi(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, t) \) requires dealing with a huge configuration space associated to the \( N \) degrees of freedom \( \vec{r}_1, \vec{r}_2, ..., \vec{r}_N \).

However, in principle, the practical computation of each Bohmian trajectory, for example \( \vec{r}_1[t] \), requires the time-integration of the Bohmian velocity \( \vec{v}(\vec{r}, \vec{r}_1[t], ..., \vec{r}_N[t], t) \) that can be obtained just from the knowledge of the conditional wavefunction, \( \Psi(\vec{r}_1, \vec{r}_2[t], ..., \vec{r}_N[t], t) \), which “lives” in a single-particle configuration space. Following this idea, it has been demonstrated in \cite{3} that a system of \( N \) interacting particles can be decomposed into \( N \) single-particle (pseudo) Schrödinger equations coupled by the \( N \) Bohmian trajectories \( \vec{r}_1[t], \vec{r}_2[t], ..., \vec{r}_N[t] \). The proposal has similarities with the original work of Kohn and Sham \cite{4} on the DFT. The formidable simplification on the many-particle computations comes at the price that some terms of the potential energy of the corresponding single-particle Schrödinger equations are unknown (the exchange correlation functional in the DFT and a complex potential energy in \cite{3}) and they have to be approximated.

The practical viability of the previously mentioned many-particle Bohmian algorithm has been demonstrated. In particular, the algorithm in \cite{3} has been used to develop a powerful quantum (Monte Carlo) simulator of electron transport for nanoelectronic devices (in time-dependent, open systems and far from equilibrium scenarios). With standard computing facilities, the present proposal is able to deal with around 100 electrons with Coulomb and exchange interactions. Numerical computations of the electron-electron correlation effects on the DC, AC and current noise in resonant tunnelling devices are presented \cite{2}\cite{5}. The application of our many-particle Bohmian algorithm into other fields (such as the study of photoionization) is in progress \cite{2}.

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Partial linearized density matrix dynamics
for dissipative, non-adiabatic quantum evolution

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An approach for treating dissipative, non-adiabatic quantum dynamics in general model systems at finite temperature based on linearizing the density matrix evolution in the forward-backward path difference for the environment degrees of freedom is presented. We demonstrate that the approach can capture both short time coherent quantum dynamics and long time thermal equilibration in an application to excitation energy transfer in a model photosynthetic light harvesting complex. The performance of the approach is also explored for a number of multidimensional multi-state model non-adiabatic relaxation problems.
Beating the efficiency of both quantum and classical simulations with semiclassics [1]

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While rigorous quantum dynamical simulations of many-body systems are extremely difficult (or impossible) due to the exponential scaling with dimensionality, corresponding classical simulations completely ignore quantum effects. Semiclassical methods are generally more efficient but less accurate than quantum methods, and more accurate but less efficient than classical methods. We find a remarkable exception to this rule by showing that a semiclassical method can be both more accurate and faster than a classical simulation. Specifically, we prove that for the semiclassical dephasing representation [1] the number of trajectories needed to simulate quantum fidelity is independent of dimensionality and also that this semiclassical method is even faster than the most efficient corresponding classical algorithm [2]. Analytical results are confirmed with simulations of quantum fidelity in up to 100 dimensions with $2^{1700}$-dimensional Hilbert space.

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Fractal Weyl law behaviour in an open Hamiltonian system

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We numerically show fractal Weyl law behavior in an open Hamiltonian system that is described by a smooth potential (rotating Henon-Heiles) and which supports numerous above-barrier resonances. This behavior holds even relatively far away from the classical limit. The complex resonance wave functions are found to be localized on the fractal classical repeller. The structure of the phase space in the repeller is also analyzed.
Phase space master equations for quantum Brownian motion in a periodic potential: 
Comparison of various kinetic models

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The dynamics of quantum Brownian particles in a cosine periodic potential are studied using the phase space formalism associated with the Wigner representation of quantum mechanics. Various kinetic phase space master equation models describing quantum Brownian motion in a potential are compared by evaluating the dynamic structure factor and escape rate from the differential recurrence relations generated by the models. The numerical solution is accomplished via matrix continued fractions in the manner customarily used for the classical Fokker-Planck equation. The results of numerical calculations of the escape rate from a well of the cosine potential are compared with those given analytically by the quantum-mechanical reaction rate theory solution of the Kramers turnover problem for a periodic potential given by Georgievskii and Pollak [Phys. Rev. E 49, 5098 (1994)], enabling one to appraise each model.
Quantum correlations and mutual synchronization

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Synchronization phenomena have been observed in a broad range of biological, chemical and physical systems, generally classical [1]. Our aim is to extend the study of this phenomenon to fundamental quantum models in order to explore possible relations with quantum effects. We consider as a prototypical model a system of coupled quantum harmonic oscillators with different frequencies and dissipating into the environment, in both the cases of common and separate baths [2].

We show that the ability of the system to synchronize depends on the existence of disparate decay rates induced by the presence of a common dissipation environment while for separate bath, independently on the strength of the oscillators coupling synchronization does not arise [3]. Further we show that this phenomenon is accompanied by robust quantum discord and mutual information between the oscillators, preventing the leak of information from the system [3]. Finally, preliminary results about generalizations to a larger number of oscillators in arrays will be discussed.


Example of dynamical evolution of the synchronization quality both for common (blue line) and separate baths (green) for temperature T = 10\omega_1 (in natural units). Perfect synchronization is reached for C=1. The insets show synchronization values when varying the ratio between frequencies and coupling between the two oscillators both for common (CB) and separate baths (SB).
How general are time-local master equations?

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Time-local master equations are convenient in many situations, for example when performing quantum trajectory simulations. Master equations in the so-called Lindblad-Kossakowski form are well understood and widely used. Time-local master equations can however be used also to describe non-Markovian behaviour. The decay rates in a Lindblad-type time-local master equation may then become time-dependent, and even negative. It is now widely accepted that negativity of decay rates is linked to non-Markovian behavior. But when the time evolution of a system becomes non-invertible, meaning that two initial states may evolve to the same state at some point in time, it is questionable whether one can use a time-local master equation to describe this evolution [1]. In this work, we investigate such a case. The master equation for a two-level atom is obtained by tracing over the field in the Jaynes-Cummings model. We show that it is possible to construct different Hamiltonians and time evolutions that lead to the same time-local master equation. These constructions are nevertheless somewhat artificial in that they involve instantaneous changes in the Hamiltonian, more specifically, instantaneous changes in the detuning and amplitude of the field. These changes must also occur at very specific times.

Green Function for the Classical and Quantum Kramers’ Turnover Problem

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Arrhenius [1] viewed a chemical reaction as very few particles from a huge assembly in a well \((N \approx 10^{24})\) escaping over a potential barrier. Particles just reaching the top can escape due to thermal agitation. The Arrhenius equation for the escape rate, \(\Gamma\), and the greatest relaxation time of a particle in the well, \(\tau\), can be found from transition state theory (TST) as

\[
\Gamma = \Gamma_{TST} = f_a e^{-\Delta V} = j/N = 1/\tau \quad (f_a \text{ is the frequency of oscillations of a particle at the bottom of the well, } \Delta V \text{ is the barrier height, } j \text{ is the current over the barrier}).
\]

By expanding \(V(x)\) about \(x = x_A\) we have

\[
f_a = \frac{1}{2\pi} \sqrt{\frac{m}{2\Delta}}
\]

which depends only on the shape of the potential. TST assumes thermal equilibrium and, accordingly, the Maxwell-Boltzmann distribution holds in the well. This is not a valid assumption as particles leaving at the well will disturb that distribution. In 1940 Kramers [2] derived a formula for \(\Gamma\) accounting for the disturbance using the theory of Brownian motion in order to represent the heat bath. Kramers was able to calculate \(\Gamma\) in two specific regions of damping: (1) Intermediate to High Damping, IHD, where

\[
\Gamma_{IHD} = \left(1 + \frac{\gamma^2}{4a_c^2} - \frac{\gamma}{2a_c}\right) \Gamma_{TST} \quad (\gamma \text{ is the friction coefficient per unit mass, } x \text{ is the position, } p \text{ is the momentum, } \omega_c \text{ is the natural angular frequency of oscillations of a particle if the potential is inverted, called the barrier frequency})
\]

and (2) Very Low Damping, VLD where

\[
\Gamma_{VLD} = \frac{\gamma}{k_B} I(E_c) \frac{a_c}{2\pi} e^{-\Delta} = \frac{\gamma}{k_B} I(E_c) \Gamma_{TST} = \Delta \Gamma_{TST} \quad (I(E_c) \text{ is the action of a particle with energy equal to the critical barrier energy over a full oscillation in the well and } \Delta \text{ is the energy loss per cycle of a librating particle with the barrier energy over the Thermal energy}).
\]

The parameter \(\Delta\) delineates the range of validity of the various asymptotic formulae for the escape rate. If \(\Delta >> 1\), IHD. If \(\Delta << 1\), VLD. Kramers was not able to solve the problem in the part of the underdamped region between ID and VLD, i.e. \(\Delta \leq 1\). This is the turnover region giving rise to Kramers’ turnover problem. Mel’nikov [3] solved this problem 50 years later. The calculations are, however, very complicated and are not readily accessible. It is the purpose of this project to try and render them in a more intelligible form in both classical and quantum cases. Mel’nikov concluded that in the classical case a single isolated well

\[
\Gamma = \left(1 + \frac{\gamma^2}{4a_c^2} \right)^{1/2} - \frac{\gamma}{2a_c} \Lambda(\Delta) \Gamma_{TST} \quad \text{where the depopulation factor,}
\]

\[
\Lambda(\Delta) = \exp \left[ \frac{1}{2\pi} \int_{+\infty}^{+\infty} e^{-\Delta} \left(\frac{\sqrt{\lambda^2 + \frac{1}{4}}}{\lambda^2 + \frac{1}{4}}\right) \lambda d\lambda \right]
\]

For HD \(\Delta >> 1\) and, therefore, \(\Lambda(\Delta) \rightarrow 1\), giving us the original IHD result, and for the VLD limit \(\Lambda(\Delta) \rightarrow \Delta\), yielding the VLD result. When Mel’nikov treated the underdamped quantum case he refers to a 1985 paper by Larkin and Ovchinnikov [4] for his method. Their paper, however, also does not contain sufficient detail. We were able to rederive the details of this paper as far as equations 17 and 18. This paper gives the details of these calculations. Our objective was to calculate equation 17, the transition probability, \(W_{jf} = \langle |A_{jf}|^2 \rangle_T\).

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Decoherence in double quantum dots

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Coherent tunnel coupling of two neighboring quantum dots represents a major achievement in mesoscopic transport. By now it is possible to capacitively couple two such mesoscopic conductors to form interacting transport channels. Recently, several experiments have been performed with both lateral and self-assembled quantum dots. In this talk, two different physical situations will be addressed: First, we consider the mutual blocking of two double quantum dots, for which a characteristic temperature-dependent shot noise has been measured. It is governed by decoherence stemming from the interaction with substrate phonons [1]. Second, if one double dot is detached from the leads, it forms a charge qubit. Then current measurements at the other double dot can be used for the readout of both the charge degree of freedom and the phase of delocalized states [2].

Coherent dynamics of electrons in ac driven quantum dot arrays

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A powerful method of manipulating the coherent dynamics of quantum particles is to control the phase of their tunneling. We will show how such phases can be produced in two distinct and complementary ways. We have considered the dynamics of two interacting electrons hopping on a quasi one-dimensional lattice with a non-trivial topology, threaded by a uniform magnetic flux, and study the effect of adding a time-periodic ac electric field. We will show that the dynamical phases produced by the driving field can combine with the familiar Aharonov-Bohm phases arising from the magnetic flux to give precise control over the dynamics and localization of the particles, even in the presence of strong particle interactions [1].

Recent electron spin resonance experiments measure coherent spin rotations of one single electron, a fundamental ingredient for quantum operations. We will show how it is possible to manipulate electron charge and spin dynamics in double and triple quantum dots by means of ac magnetic fields. We demonstrate that by tuning the ac magnetic fields parameters, i.e., the field intensity, frequency and the phase difference between the fields within each dot, coherent destruction of tunneling (and thus charge localization) can be achieved. We show that in contrast with ac electric fields, ac magnetic fields are also able to induce spin locking, i.e., to freeze the electronic spin, at certain field parameters [2]. Spin Blockade has been measured in transport experiments through double and triple quantum dots. We will discuss the effect of ac magnetic fields on Spin Blockade and we will show that it can not only be removed by external ac magnetic fields, but also it can be induced at certain parameters of the field [3].

Towards decoherence studies in optical microfibers

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The discussions of the fundamental status of quantum mechanics have largely been centred around the Einstein-Podolsky-Rosen (EPR) paradox and the Schrödinger cat paradox\,[1]. Causality and non-locality, the main topics of the Bohr-Einstein dispute, were considered at time by most a philosophical topic. However, since Bell published the famous inequalities, and Aspect subjected these to experimental tests, it was clear that the collected experimental evidence definitely shifted focus, both on the importance in terms of quantum mechanics, as on the concept of entanglement.

On the other side, this final link to solve the Schrödinger cat paradox is not yet available. The quantum measurement problem, including both the wavefunction collapse vs. decoherence dispute, as well as the unambiguous identification of a quantum-to-classical threshold, consists, and it has to be taken for granted that the further collection of experimental evidence will be fundamental if any broader consensus concerning this question is to be achieved. Towards a proper clarification of this question, recent advancements of both experimentalist\,[2] as theorist\,[3] have significantly contributed.

The purpose of this paper is to share with the audience a concept that could eventually lead to decoherence studies with entangled photons. It is foreseen to be integrated and executed within an experimental setup that produces entangled photons obtained by parametric down conversion in two adjacent thin BBO crystals. We will discuss the experiments of the twin photon pairs propagating inside tapered optical micro- and nanofibers. The manufactured tapered fibers, obtained by the flame-brushing technique, offer the possibility to engineer precisely the local fiber radius length scale, associated to the transverse confinement of the photons. Hence, coupling and effective propagation constants can be adequately engineered, for example into interferometric structures\,[4]. It will be discussed in how far this measurement architecture could be employed, in principle, to study the decoherence issue.

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Decay and entanglement with reservoir structures

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Static reservoir structures coupled to simple quantum systems can be analysed by the method of “pseudomodes”, where the reservoir structure is replaced by an effective mode [1]. The approach can be useful for strongly coupled, i.e. non-Markovian problems. A brief introduction to this theory will be given together with recent results on reservoir memory [2] and entanglement in the reservoir [3].


*Work performed together with: I. Yu. Sklyadneva, E. V. Chulkov and P. M. Echenique (DIPC and UPV, Donostia/San Sebastián, Spain); R. Heid K.-P. Bohnen (Forschungszentrum Karlsruhe, Germany); J. P. Toennies (MPI-DS, Goettingen, Germany).
Hierarchical effective mode approach to non-Markovian reduced dynamics

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The talk will focus on our recent developments of a hierarchical effective mode approach to quantum dynamics. The approach is based on a transformation of a large dimensional system, typically a bath, into a series of effective modes. It is shown that the short-time dynamics is entirely accounted for by the effective modes. Furthermore, inclusion of residual modes bilinearly coupled in a Mori chain type description successively accounts for the dynamics over longer time-scales. Termination of the chain by coupling the final member of the chain to a Markovian bath yields a general representation of non-Markovian system-bath dynamics.

We have further shown that Markovian closure of the chain at successive orders generates a family of approximate spectral densities which approach the true spectral density with increasing accuracy [1-4]. The approach has recently been applied to the study of exciton dissociation at interfaces of semiconducting polymers [5,6].

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