Titles and Abstracts

Talks

Lajos Diosi

Wigner Research Centre for Physics, Budapest, Hungary

Hybrid dynamics of a quantum and a canonical classical subsystem

Quantum-classical hybrid dynamics cannot retain the reversibility of the constituent quantum and classical dynamics. If, for instance, the classical constituent is canonical and we construct a deterministic hybrid dynamics using the sum of the Dirac and Poisson brackets, the positivity of the hybrid density is not preserved. For a legitimate Markovian dynamics, we should impose additional decoherence and diffusion mechanisms respectively on the quantum and classical evolutions. It turns out that the product of the decoherence and diffusion coefficients cannot be smaller than the strength of hybrid coupling. This implies a condition for the minimum of the mandatory irreveribility of hybrid dynamics.

Rosario Lo Franco

Engineering Department, University of Palermo, Italy

General robust preparation of maximally entangled states via identical particle interferometry

Realistic preparations of entangled states are jeopardized by the unavoidable interaction with the surrounding environment, whose noisy action is detrimental for the quantum correlations within the system. For this reason, many different techniques to circumvent the problem have been proposed over time.

We present a general scheme, valid for both bosons and fermions, to prepare maximally entangled states of two identical qubits in a way that is robust under the effect of any type of local noise, both quantum and classical. Considering linear optics operations, the procedure utilizes an externally-activated depolarizing channel and a pseudospin-insensitive, non-absorbing, parity check detector in an iterative process with probability which converges exponentially to one with the number of repetitions. The scheme is thus asymptotically deterministic. Distributing the particles over two distinct spatial modes, we further show that the elements of the basis composed of maximally entangled states can be divided in two sets according to an equivalence based on passive optical transformations. We demonstrate that the parity check detector can be used to connect these two sets of states.

The proposed procedure can be ultimately exploited to prepare any pure state of two identical qubits which are maximally entangled in either the internal degree of freedom (Bell states) or the spatial mode (NOON states).

Marcel Reginatto[1], Andrés Bermudez Manjarres[2], Sebastian Ulbricht[1]

[1]Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany

[2]Universidad Distrital Francisco José de Caldas, Cra 7 No. 40B-53, Bogotá, Colombia

On connections between three different models of hybrid quantum-classical systems

A number of issues arise when modelling the interaction of classical and quantum systems. It becomes necessary to find a common mathematical framework, which is not straightforward

as the usual formulations of classical and quantum mechanics are based on very different mathematical structures. In addition, there are conceptual issues related to the way in which we define “classical” and “quantum” which play a role when choosing the properties of classical and quantum mechanics which should be preserved when these systems interact. Different approaches are possible depending on how these issues are handled. We contrast three hybrid quantum-classical models: configuration- and phase-space ensemble approaches and a Hilbert space approach. Our main aim is to look at the connections between these different models. To do this, we examine the extent to which it is possible to establish equivalence of states, equations of motion, observables, and generators. Despite many common features, we find that there are important differences between the approaches.

Giovanni Manfredi

Institut de Physique et Chimie des Matériaux de Strasbourg
Centre National de la Recherche Scientifique and Université de Strasbourg, France

Quantum control of gravitationally-bound ultracold neutrons

Ultracold neutrons confined in the Earth’s gravitational field display quantized energy levels that have been observed for over two decades [1]. In recent resonance spectroscopy experiments [2], the transitions between two such gravitational quantum states were driven by the mechanical oscillation of the plates that confine the neutrons. Here, we show that by applying a sinusoidal modulation with slowly varying frequency (chirp), the neutrons can be brought to higher excited states by climbing the energy levels one by one [3]. The proposed experiment should make it possible to observe the quantum/classical transition that occurs at high neutron energies. Furthermore, it provides a technique to realize superpositions of gravitational quantum states, to be used for precision tests of gravity at short distances.

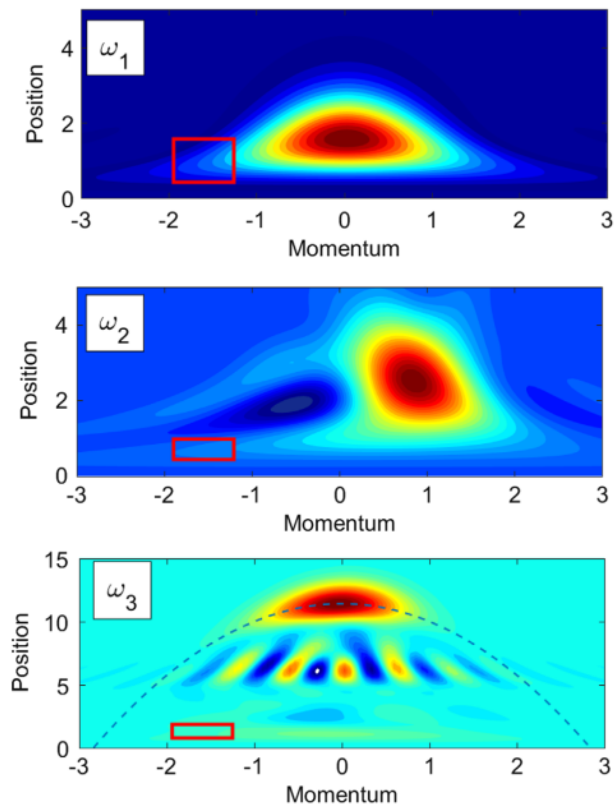

FIG. 2. Wigner functions in the phase space (x, p) at three different times corresponding to the three frequencies $\omega_{1,2,3}$ shown in Fig. 1. The red rectangle shows a phase-space area equal to $\hbar$. In the bottom panel, the dashed line shows the corresponding classical trajectory. Position and momentum are expressed in normalized units.

[1] V. V. Nesvizhevsky et al., Nature **415**, 297 (2002).

[2] T. Jenke et al., Nat. Phys. **7**, 468 (2011).

[3] G. Manfredi, O. Morandi, L. Friedland, T. Jenke, H. Abele, Phys. Rev. D **95**, 025016 (2017).

Ahsan Nazir

Department of Physics and Astronomy, University of Manchester, UK

Quantum work statistics at strong reservoir coupling

Calculating the stochastic work done on a quantum system while strongly coupled to a reservoir is a formidable task, requiring the calculation of the full eigenspectrum of the combined system and reservoir. In this talk I will show that this issue can be circumvented by using a polaron transformation that maps the system into a new frame where weak-coupling theory can be applied. It is shown that the work probability distribution is invariant under this transformation, allowing one to compute the full counting statistics of work at strong reservoir coupling. Crucially this polaron approach reproduces the Jarzynski fluctuation theorem, thus ensuring consistency with the laws of stochastic thermodynamics. I will apply the formalism to a system driven across the Landau-Zener transition, where clear signatures in the work distribution arising from a non-negligible coupling to the environment are identified. These results provide a new method for studying the stochastic thermodynamics of driven quantum systems beyond Markovian, weak-coupling regimes.

Dorje Brody

School of Mathematics and Physics, University of Surrey, UK

A Hilbert space approach to cognitive psychology (Special Templeton Talk)

The cognitive state of mind concerning a range of choices to be made can effectively be modelled in terms of an element of a high-dimensional Hilbert space. The dynamics of the state of mind resulting form information acquisition is characterised by the von Neumann-Lüders projection postulate of quantum theory. This gives rise to an uncertainty-minimising dynamical behaviour, classically equivalent to the Bayesian updating and quantum mechanically leading to the Lindblad dynamics of open quantum systems, hence providing an alternative approach to characterising the dynamics of cognitive state that is consistent with the free energy principle in brain science. The quantum formalism however goes beyond the range of applicability of classical reasoning in explaining cognitive behaviours, thus opens up new and intriguing possibilities. I will speculate that any artificial intelligence architecture based on classical probabilistic reasoning will ultimately be unable to accurately replicate human thinking, whereas an ‘artificial quantum intelligence’, implementing the von Neumann-Lüders rule and open quantum dynamics, will go a long way.

Posters

Paul Bergold and Cesare Tronci

School of Mathematics and Physics, University of Surrey, UK

Simulating Mixed Quantum-Classical Dynamics Using the Koopmon Method

Mixed quantum-classical models have been proposed in several contexts to overcome the computational challenges of fully quantum approaches. However, current models typically suffer from long-standing consistency issues, and, in some cases, invalidate Heisenberg's uncertainty principle. Here, we present a fully Hamiltonian theory of quantum-classical dynamics that appears to be the first to ensure a series of consistency properties, beyond positivity of quantum and classical densities. We also exploit Lagrangian trajectories to formulate a finite-dimensional closure scheme for numerical implementations, the 'koopmon method', and a few benchmark case studies are presented.

Adam Burgess,[1, 2] Marian Florescu,[2] and Dominic M. Rouse[3, 4]

[1]*Leverhulme Quantum Biology Doctoral Training Centre, University of Surrey, Guildford, GU2 7XH, UK*
[2]*Department of Physics and Advanced Technology Institute, University of Surrey, Guildford, GU2 7XH, UK*
[3]*School of Physics and Astronomy, University of Glasgow, Glasgow G12 8QQ, Scotland, UK*
[4]*Department of Physics and Astronomy, University of Manchester, Oxford Road, Manchester M13 9PL, UK*

Strong coupling dynamics of driven quantum systems with permanent dipoles

Many optically active systems possess spatially asymmetric electron orbitals. These generate permanent dipole moments, which can be stronger than the corresponding transition dipole moments, significantly affecting the system dynamics and creating polarised Fock states of light. We derive a master equation for these systems with an externally applied driving field by employing an opti- cal polaron transformation that captures the photon mode polarisation induced by the permanent dipoles. This provides an intuitive framework to explore their influence on the system dynamics, the driving and emission spectrum. We find that permanent dipoles introduce multiple-photon processes and a photon sideband which causes substantial modifications to single-photon transition dipole pro- cesses. In the presence of an external drive, permanent dipoles lead to an additional process that we show can be exploited to optimise the decoherence and transition rates. We derive the emission spectrum of the system, highlighting experimentally detectable signatures of optical polarons, and measurements that can identify the parameters in the system Hamiltonian, the magnitude of the differences in the permanent dipoles, and the steady-state populations of the system.

Lester Buxton, Marc-Thomas Russo, Jim Al-Khalili, Andrea Rocco (Surrey)

School of Mathematics and Physics & Leverhulme Quantum Biology Doctoral Training Centre, University of Surrey, GU2 7XH, Guildford, UK

Quantum Brownian Motion in the Caldeira-Leggett Model with a Damped Environment

We model a quantum system coupled to an environment of damped harmonic oscillators by following the approach of Caldeira-Leggett and adopting the Caldirola-Kanai Lagrangian for the bath oscillators. In deriving the master equation of the quantum system of interest (a particle in a general potential), we show that the potential is modified non-trivially by a new inverted harmonic oscillator term, induced by the damping of the bath oscillators. We analyze numerically the case of a particle in a double-well potential and find that this modification changes both the rate of decoherence at short times and the well-transfer probability at longer times. We also identify a simple rescaling condition that keeps the potential fixed despite changes in the environmental damping. Here, the increase of environmental damping leads to a slowing of decoherence. The complete work can be found in [1].

[1] Buxton, L., Russo, M.-T., Al-Khalili, J., & Rocco, A. (2023). Quantum Brownian Motion in the Caldeira-Leggett Model with a Damped Environment. arXiv preprint arXiv:2303.09516.

Robson Christie and Eva-Maria Graefe

Department of Mathematics, Imperial College London, UK

Modified Caldeira-Leggett Oscillator Dynamics at Low Temperatures

We present a modified Caldeira-Leggett Lindblad dynamics for the harmonic oscillator at low temperatures. By ensuring that these modified Lindblad dynamics preserve the thermal state at all temperatures and asymptotically approach the standard form in the high-temperature regime, we derive a model for quantum Brownian motion in a Harmonic oscillator. Furthermore, we show that in the classical limit, the modified Lindblad equation and its stochastic Schrödinger unraveling converge to the standard Fokker-Planck and Langevin dynamics, respectively.

Thomas Guff and Andrea Rocco

School of Mathematics and Physics, University of Surrey, UK

Time reversal symmetry in open classical and quantum systems

We follow several standard derivations of irreversible Markovian dynamics from open system models which begin time reversal symmetric, to examine which assumption breaks time reversal symmetry. In particular, we examine the Ohmic approximation in the Caldeira-Leggett model to derive the Langevin equation. We find that this approximation does not destroy time reversal symmetry, with the resulting Langevin equation showing thermalisation into the future as well as into the past. This symmetry propagates into the subequent Fokker-Planck, and Brownian motion master equations. This is also true for standard derivations of the Lindblad equation and the Pauli master equation. These equations thus predict dynamics which is Markovian into the past and the future from the temporal origin.

Jesus Rubio Jimenez

School of Mathematics and Physics, University of Surrey, UK

Quantum scale metrology: measuring the lifetime of a mixed state

Progress across modern quantum sciences, from fundamental aspects to technological developments, is intimately connected to the possibility of performing highly precise measurements. This has led to a careful revision of the foundations of metrology beyond phase estimation, enabling the access to new regimes including dissipative dynamics, finite information, incompatible estimators, and parameters other than phases. This poster presents the optimal quantum strategy - estimator, POVM, and ultimate precision limit - for the measurement of time scales of dissipative processes. Spontaneous photon emission is chosen as the case study. This is achieved by means of quantum scale metrology, a new Bayesian framework based on logarithmic errors that enables the precise estimation of scale parameters.

J. Rubio, Quantum Sci. Technol. 8 015009 (2022)

R. Demkowicz-Dobrzański, W. Górecki and M. Guţă, J. Phys. A: Math. Theor. 53 363001 (2020)

Louie Slocombe[1], Max Winokan[2], Jim Al-Khalili[3], Marco Sacchi[2]

1 Department of Chemistry, University of Surrey, UK
2 Leverhulme Quantum Biology DTC, University of Surrey, UK

3 Department of Physics, University of Surrey, UK

Quantum Tunnelling Effects in the Guanine-Thymine Wobble Misincorporation via Tautomerism

DNA polymerase is an enzyme that catalyzes the synthesis of DNA molecules by matching complementary deoxyribonucleoside triphosphates (dNTP) to the template DNA strand using the standard Watson–Crick base pair rules. However, when a noncomplementary dNTP diffuses into the active site during the polymerase dNTP sampling, the polymerase domain will transition from an open to an ajar conformation, thus forming a different nonstandard hydrogen-bonded base-pairing arrangement called wobble mispair [1]. While there are other sources of replication errors, the fidelity of replication primarily depends on the ability of polymerases to select and incorporate the correct complementary base [2].

Consequently, misincorporating a noncomplementary DNA base in the polymerase active site is a critical source of replication errors that can lead to genetic mutations [3]. In this work [4], we model the mechanism of wobble mispairing and the subsequent rate of misincorporation errors by coupling first-principles quantum chemistry calculations to an open quantum systems master equation [5]. This methodology allows us to accurately calculate the proton transfer between bases, allowing the misincorporation and formation of mutagenic tautomeric forms of DNA bases. Our calculated rates of genetic error formation are in excellent agreement with experimental observations in DNA. Furthermore, our quantum mechanics/molecular mechanics model predicts the existence of a short-lived "tunnelling-ready" configuration along the wobble reaction pathway in the polymerase active site, dramatically increasing the rate of proton transfer by a hundredfold, demonstrating that quantum tunnelling plays a critical role in determining the transcription error frequency of the polymerase.

[1] Wang, W., Hellinga, H. W., & Beese, L. S. (2011). Proceedings of the National Academy of Sciences, 108(43), 17644-17648.

[2] Kimsey, I. J., Szymanski, E. S., Zahurancik, W. J., Shakya, A., Xue, Y., Chu, C. C., ... & Al-Hashimi, H. M. (2018). Nature, 554(7691), 195-201.

[3] Li, P., Rangadurai, A., Al-Hashimi, H. M., & Hammes-Schiffer, S. (2020). Journal of the American Chemical Society, 142(25), 11183-11191.

[4] Slocombe, L., Winokan, M., Al-Khalili, J., & Sacchi, M. (2022). The Journal of Physical Chemistry Letters, 14, 9-15.

[5] Slocombe, L., Sacchi, M., & Al-Khalili, J. (2022). Communications Physics, 5(1), 1-9.