DY 4: Poster Session II: Nonlinear Dynamics, Simulations and Machine Learning

Time: Tuesday 17:30–19:30 Location: P

DY 4.1 Tue 17:30 P

Memory effects and stochastic forces on a passive particle in an active bath — •Jeanine Shea[1], Friederike Schmid[1], and Gerhard Jung[2] — [1]Johannes Gutenberg University — [2]University of Innsbruck

Implicit models of passive, equilibrium systems have been used for many years to study and understand the physical behavior of these systems. Given the success of understanding equilibrium systems through models, recent studies have focused on mapping non-equilibrium systems onto modified equilibrium models to better understand non-equilibrium behavior. In particular, active systems are non-equilibrium systems which are highly pertinent to biological studies and which exhibit vastly different behavior than strictly passive systems. These distinctive dynamics are not limited to purely active systems, but can also be transferred to passive particles in active systems. As such, the behavior of passive particles immersed in active systems can significantly differ from that in a passive system. We investigate the dissipative and stochastic forces which act on one fundamental example of such a system, that of a colloid in a bath of active particles.

DY 4.2 Tue 17:30 P

Epidemic modeling with delay-differential equations including saturation effects by isolation and contact restriction — •Susanne Kiefer and Edeltraud Gehrig — RheinMain University of Applied Science, Germany

Delay differential equation enable a realistic modeling of epidemics since they allow the inclusion of incubation periods, recovery times or the influence of a quarantine. A systematic modelling of the influence of parameters and their mutual dependence is of high importance when analyzing the behavior of the numbers of infected, susceptible and recovered persons. In this work we present and compare epidemic models with variable delays and saturation parameters. Thereby we consider both, a delay term describing the influence of incubation time as well as a delay for an inclusion of recovery. Our stability analysis and modeling of the temporal behavior allow for a determination of critical regimes where, depending on model approach, a delay may turn the system into instable behavior. A rise in amplitude of the characteristic oscillations shows a strong dependence on delay. This behavior may be controlled by parameters describing quarantine rules. Results of our simulations reveal an influence of parameters describing isolation of infected persons and contact restrictions on the dynamics and particularly on the transition to unstable behavior. A thorough adjustment of contact restriction and isolation may allow to shift the onset of instability and to adjust restriction rules. Thereby the range of control options of each of these parameters critically depends on initial values, infection and recovery rates as well on the delays.

DY 4.3 Tue 17:30 P

Interplay of viscosity and surface tension for ripple formation by external laser melting — •Klaus Morawetz[1,2], Sarah Trinschek[1], and Evgeny Gurevich[1] — [1]Münster University of Applied Sciences,Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [2]International Institute of Physics- UFRN,Campus Universitário Lagoa nova,59078-970 Natal, Brazil

A model for ripple formation on liquid surfaces exposed to an external laser or particle beam and a variable ground is developed. Starting from the Navier Stokes equation the coupled equations for the velocity potential and the surface height are derived with special attention to viscosity. Linear stability analysis provides the formation of a damped gravitation wave modified by an interplay between the external beam, the viscosity, and the surface tension. The resulting wavelengths are in the order of the ripples occurring in laser welding experiments hinting to their hydrodynamical origin. The stability due to the periodic time-dependence of the external beam is discussed with the help of Floquet multipliers showing that the ripple formation could be triggered by an external excitation with frequencies in the order of the repetition rate of the laser. The weak nonlinear stability analysis provides ranges where hexagonal or stripe structures can appear. The orientation of stripe structures and ripples are shown to be dependent on the incident angle and a minimal angle is reported. Two models are presented to couple the external current to the gradient of the surface. Numerical simulations confirm the findings. arXiv:2107.02651

DY 4.4 Tue 17:30 P

Observation of phase synchronization and alignment during free induction decay of quantum spins with Heisenberg interactions — •Patrick Vorndamme[1], Heinz-Jürgen Schmidt[2], Christian Schröder[1,3], and Jürgen Schnack[1] — [1]Bielefeld University, 33615 Bielefeld, Germany — [2]Osnabrück University, Barbarastraße 7, 49076 Osnabrück, Germany — [3]Bielefeld Institute for Applied Materials Research, 33619 Bielefeld, Germany

Equilibration of observables in closed quantum systems that are described by a unitary time evolution is a meanwhile well-established phenomenon. Here we report the surprising theoretical observation that spin rings with nearest-neighbor or long-range isotropic Heisenberg interaction not only equilibrate but moreover also synchronize the directions of the expectation values of the individual spins. Here, we observe mutual synchronization of local spin directions in closed systems under unitary time evolution. This synchronization is independent of whether the interaction is ferro- or antiferromagnetic. In our numerical simulations, we investigate the free induction decay of an ensemble of quantum spins by solving the time-dependent Schrödinger equation numerically exactly. The synchronization is very robust against for instance random fluctuations of the Heisenberg couplings and inhomogeneous magnetic fields. Synchronization is not observed with strong enough symmetry-breaking interactions such as the dipolar interaction. We also compare our results to closed-system classical spin dynamics which does not exhibit phase synchronization due to the lack of entanglement. (arxiv:2104.05748)

DY 4.5 Tue 17:30 P

Neural Network-Based Approaches for Multiscale Modelling of Topological Defects — •Kyra Klos[1], Karin Everschor-Sitte[2], and Friederike Schmid[1] — [1]Johannes Gutenberg University, Mainz, Germany — [2]University of Duisburg-Essen, Duisburg, Germany

Topological defects and their dynamics are a heavily researched topic in a wide range of physics fields.[1]

Due to the multiscale character of those defect structures, numerically simulating a large number of them in full microscopic detail gets highly complicated, as the large size of associated deformation fields around each core leads to a complex interaction pattern.

To give a possible insight into the connection between the macroscopic (particle) description of a model with topological defects and the underlying microscopic true structure, the use of neural networks is proposed. Starting with a spin-dynamic simulated microscopic model as input [2,3], a fully convolutional network (FCN)[4] is used to simplify the complex defect structure of the microscopic theory without loss of valuable information. This allows the extraction of the configuration and location of the topological defects.

[1] Mermin, N. D., Rev. Mod. Phys. 51, 591, (1979)
[2] Leoncini, X. et. al., Phys. Rev. E 57(6), 6377, (1998)
[3] Cerruti-Sola, M. et. al., Phys. Rev. E 61(5A), 5171, (2000)
[4] Long, J. et. al., IEEE, 39(4), 640, (2017)

DY 4.6 Tue 17:30 P

Nonlinear dynamics in intra-cavity pumped thin-disk lasers — •Sarah Trinschek, Christian Vorholt, and Ulrich Wittrock — Münster University of Applied Sciences, Germany

For an intra-cavity pumped Yb:YAG thin-disk laser, complex dynamics of the laser output power can be observed. The gain medium of this laser is residing in the resonator of a conventional, diode-pumped Yb:YAG thin-disk laser. We present illustrative experimental results and a detailed analysis of the nonlinear dynamics of the laser in the framework of a rate-equation model. Despite stable continuous-wave pumping, periodic pulse trains and chaotic fluctuations of the optical power of both lasers occur. The dynamics is not driven by external perturbations but arises naturally in this laser system due to cross-saturation effects of the two gain media. The qualitative type of dynamics can be controlled by the resonator length of the diode-pumped laser but the detailed behaviour of the laser is complex and also shows hysteresis and multistability.

DY 4.7 Tue 17:30 P

Quantitative Waveform Sampling on Atomic Scales — Do-

minik Peller[1], Carmen Roelcke[1], •Lukas Kastner[1], Thomas Buchner[1], Alexander Neef[1], Johannes Hayes[1], Franco Bonafé[2], Dominik Sidler[2], Michael Ruggenthaler[2], Angel Rubio[2,3,4], Rupert Huber[1], and Jascha Repp[1] — [1]University of Regensburg, Germany — [2]MPSD, MPG, Hamburg, Germany — [3]CCQ, Flatiron Institute, New York, USA — [4]UPV/EHU, San Sebastían, Spain

Using a single molecule as a local field sensor, we precisely sample the absolute field strength and temporal evolution of tip-confined near-field transients in a lightware-driven scanning tunnelling microscope. To develop a comprehensive understanding of the extracted atomic-scale nearfield, we simulated the far-to-near-field transfer with classical electrodynamics and include time-dependent density functional theory to validate our calibration and conclusions.

DY 4.8 Tue 17:30 P

Calculating Raman Spectra using Kernel-Based Machine Learning — •Manuel Grumet[1], Karin S. Thalmann[1], Tomáš Bučko[2,3], and David A. Egger[1] — [1]Technical University of Munich, Germany — [2]Comenius University in Bratislava, Slovakia — [3]Slovak Academy of Sciences, Slovakia

First-principles theoretical predictions of Raman spectra are possible using either a phonon-based approach or molecular dynamics (MD) simulations. In both cases, the polarizability tensor of the system, α, is the central quantity. Specifically, the Raman spectrum is obtained from Fourier-transformed velocity autocorrelation functions (VACs) of tensor invariants of α in the MD method [1]. This requires a large number of evaluations of α and thus leads to high computational cost.

We use kernel-based machine learning (ML) to reduce the number of polarizability calculations needed. In this approach, a subset of all configurations serves as a training data set, and polarizabilities for all other configurations are predicted using ML methods. In particular, we obtain the polarizabilites using kernel ridge regression with descriptors based on the atomic neighbourhood density around each atom [2,3].

We apply these methods to a number of test systems, consisting of small molecules and simple solids. We compare different descriptors with regard to the size of the training data set required to obtain accurate predictions for polarizabilties and Raman spectra.

[1] M. Thomas et al., Phys. Chem. Chem. Phys. **15**, 6608 (2013)
[2] N. Raimbault et al., New J. Phys. **21**, 105001 (2019)
[3] A. P. Bartók et al., Phys. Rev. B **87**, 184115 (2013)

DY 4.9 Tue 17:30 P

Machine learning generators of open system Lindblad dynamics — •Francesco Carnazza[1], Dominik Zietlow[2], Federico Carollo[1], Sabine Andergassen[1], Georg Martius[2], and Igor Lesonovsky[1,3] — [1]Institut für Theoretische Physik and Center for Quantum Science, Universität Tübingen, Auf der Morgenstelle 14, 72076 Tübingen, Germany — [2]Max Planck Institute for Intelligent Systems, Max-Planck-Ring 4, 72076 Tübingen, Germany — [3]School of Physics and Astronomy, University of Nottingham, Nottingham, NG7 2RD, UK

In recent years artificial neural network methods have established themselves as a versatile tool to encode the state of both closed and open quantum systems. We are interested in the question whether they can learn the generator of an effective open quantum dynamics which governs a small system of interest that is embedded within a larger one (Paolo Mazza et al. 2020 https://doi.org/10.1103/PhysRevResearch.3.023084). The model we consider is a spin chain where the system of interest is formed by two spins which are coupled to a "bath" consisting of the rest of the chain. The whole chain is evolved according to an transverse field Ising Hamiltonian. From the reduced density matrix, obtained by tracing out the bath degrees of freedom, the two-body correlations are determined, which are subsequently used to train the network. A simple architecture is adopted in order to have the possibility to "look inside" the network and to see whether the learned dynamics is indeed governed by a time-local Lindblad generator.

DY 4.10 Tue 17:30 P

Modelling a highly adaptive, nonlinear acoustic sensor — •Philipp Hövel[1], Thomas Meurer[2], Martin Ziegler[3], and Claudia Lenk[3] — [1]University College Cork, Ireland — [2]Kiel University, Germany — [3]Technische Universität Ilmenau, Germany

Hearing is a remarkable sense both in terms of physiology and signal processing. In biology, hearing exhibits amazing sensing properties, in particular for low-volume sounds and noisy environments, which is known as the "cocktail party effect". For many state-of-the-art technological implementations, speech recognition remains a challenging task in these hard-to-hear situations and varying surroundings.

In this contribution, we present a mathematical model of a novel, adaptive, bio-inspired acoustic sensor with integrated signal processing functionality, whose sensing and processing properties can be widely tuned using real-time feedback. We show that dynamical switching between linear and nonlinear characteristics improves detection of signals in noisy conditions, increases the dynamic range of the sensor, and enables adaptation to changing acoustic environments. We demonstrate that the dynamical switching can be attributed to a Hopf bifurcation, and its dependence of sensor and feedback parameters is validated in experiments, and highlight the applicability and conceptual advantages of the acoustic sensor.