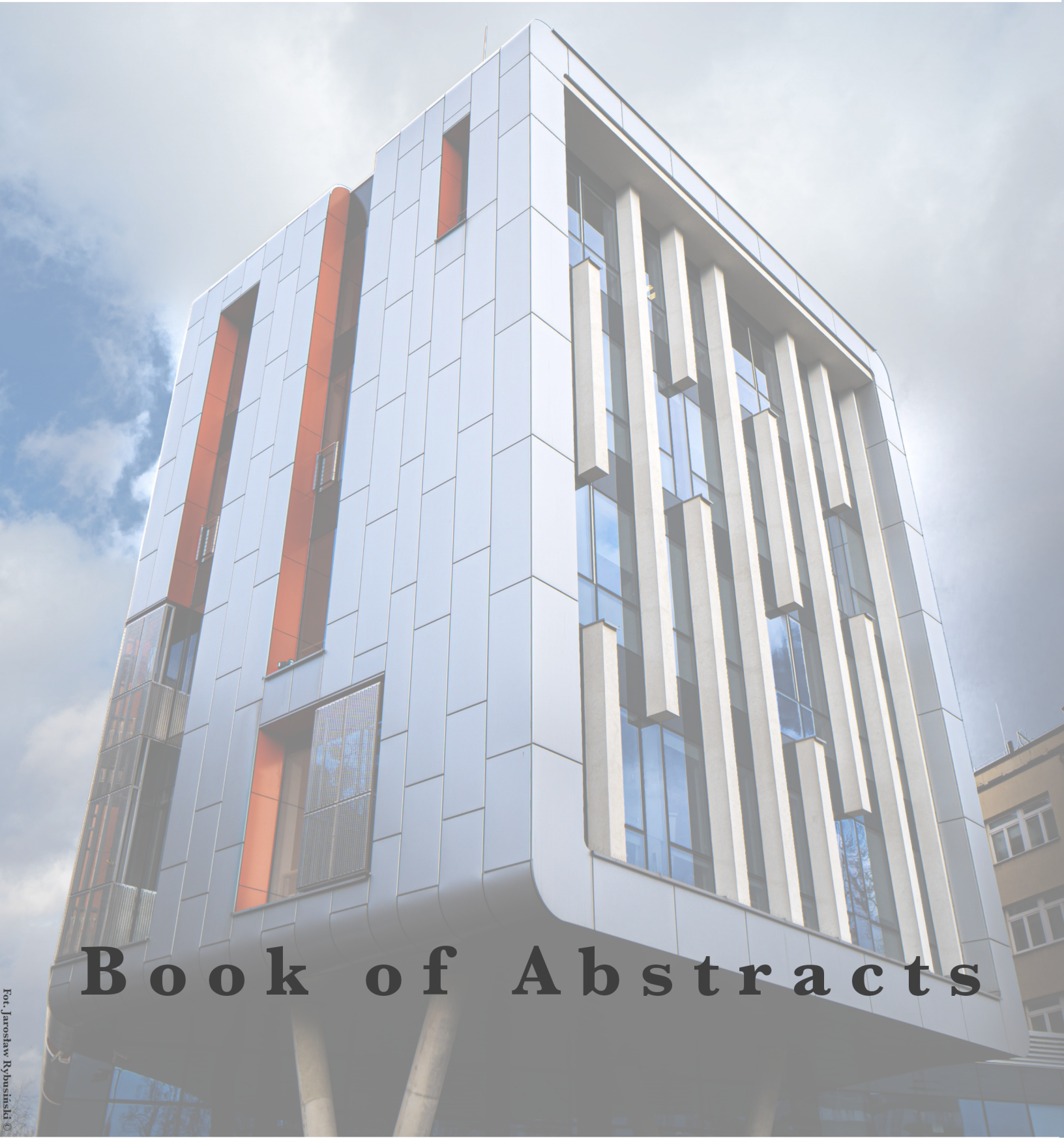
Summer School: Machine Learning In Quantum Physics and Chemistry



Book of Abstracts

Fot. Jarosław Rybusiński ©

EXCELLENCE INITIATIVE RESEARCH UNIVERSITY

UNIVERSITY OF WARSAW

MACHINE LEARNING Science and Technology

FACULTY OF PHYSICS UNIVERSITY OF WARSAW

Summer School: Machine Learning in Quantum Physics and Chemistry

24th August - 3rd September 2021, Warsaw

	Tues, 24 Aug	Wed, 25 Aug	Thurs, 26 Aug	Fri, 27 Aug	Sat, 28 Aug
9:00-11:00	Eliška Greplová (1)	Roman Krems* (1) Vancouver: 0:00-2:00	Roman Krems* (2) Vancouver: 0:00-2:00	Roman Krems* (3) Vancouver: 0:00-2:00	10:00-11:00 Yadong Wu* Stefano Mangini*
11:00-11:30	coffee break				
11:30-13:30	Eliška Greplová (2)	Eliška Greplová (3)	Evert van Nieuwenburg*	Rafał Mirek Borja Requena Pozo Aikaterini Gratsea Lorenzo Cardarelli	*hands-ons B* (Gaussian processes)
13:30-15:00	lunch				
15:00-17:00	Juan Carrasquilla* Toronto: 9:00-11:00	Alba Cervera-Lierta	free afternoon	15:30-16:00 30 flash talks 16:00-17:00 MLST: How to publish?	Sebastian Wetzel
17:00-17:30	coffee break			coffee break	
17:30-19:00	30 flash talks + poster session	*hands-ons A* (phase classification)	19:30 - dinner	poster session	

	Mon, 30 Aug	Tues, 31 Aug	Wed, 1 Sept	Thurs, 2 Sept	Fri, 3 Sept
9:00-11:00	Giuseppe Carleo* (1)	Lei Wang* Beijing: 15:00-17:00	Giuseppe Carleo* + Filippo Vicentini (3)	Florian Marquardt (2)	*hands-ons D* (reinforcement learning)
11:00-11:30	coffee break				
11:30-13:30	Patrick Huembeli	Giuseppe Carleo* (2)	Florian Marquardt (1)	12:00-13:30 Chenfeng Cao* Axel Lode* Ivan Panadero Muñoz	Florian Marquardt (3) + goodbye
13:30-15:00	lunch				
15:00-17:00	Marylou Gabrie* New York: 9:00-11:00	Vedran Dunjko* + Sofiene Jerbi*	free afternoon	Adrian Roitberg* Gainesville: 9:00-11:00	
17:00-17:30	coffee break			coffee break	
17:30-19:00	30 flash talks + poster session	*hands-ons C* (Q. Neural States)	19:00 - drinks	17:30-18:30 L.-Y. Chih* Alexander Gresch	

*online participation

EXCELLENCE INITIATIVE RESEARCH UNIVERSITY

UNIVERSITY OF WARSAW

MACHINE LEARNING Science and Technology

FACULTY OF PHYSICS UNIVERSITY OF WARSAW

Chapter 1

Contributing Speakers

Certificates of many-body quantum properties assisted by machine learning

Borja Requena Pozo

ICFO - The Institute of Photonic Sciences, Castelldefels, Spain

Contributing Speaker #1

In physics and optimization, computationally intractable tasks are often encountered. Among the various approaches to tackle such problems, relaxation techniques have been proposed to approximate the feasible set from outside, leveraging efficient descriptions of the relaxed set, thus providing bounds to the optimal solution. In this work, we propose a novel approach combining the power of relaxation techniques with deep reinforcement learning to find the best possible bounds within a limited computational budget. We illustrate the viability of the method in the context of finding the ground state energy of many-body quantum systems, a paradigmatic problem in quantum physics. We benchmark our approach against other classical optimization algorithms and we characterize the effect of transfer learning to find it may be indicative of phase transitions, with a completely unsupervised approach. Finally, we provide the tools to generalize the approach to other common applications in the field of quantum information processing.

Quantum imaginary time evolution steered by reinforcement learning

Chenfeng Cao

The Hong Kong University of Science and Technology

Contributing Speaker #2

Quantum imaginary time evolution is a powerful algorithm to prepare ground states and thermal states on near-term quantum devices. However, algorithmic errors induced by Trotterization and local approximation severely hinder its performance. Here we propose a deep-reinforcement-learning based method to steer the evolution and mitigate these errors. In our scheme, the well-trained agent can find the subtle evolution path where most algorithmic errors cancel out, therefore enhance the recovering fidelity. We verified the validity of the method with transverse-field Ising model and graph maximum cut problem. The efficacy was illustrated by numerical calculations and experiments on a nuclear magnetic resonance quantum computer. The philosophy of our method, eliminating errors with errors, sheds new light on error reduction on near-term quantum devices.

Quantum autoencoders for quantum error correction

Lorenzo Cardarelli

Forschungzentrum Jülich

Contributing Speaker #3

The operation of reliable large-scale quantum computers will foreseeably require quantum error correction procedures, in order to cope with errors that dynamically occur during storage and processing of fragile quantum information. Classical machine learning approaches, e.g. neural networks, have been proposed and successfully used for flexible and scalable strategies for quantum error correction. Complementary to these efforts, we investigate the potential of quantum machine learning for quantum error correction purposes. Specifically, we show how quantum neural networks, in the form of quantum auto-encoders, can be trained to learn optimal strategies for active detection and correction of errors, including bit-flip, depolarizing or correlated noise, or even the loss of qubits. We highlight that the denoising possibilities of quantum auto-encoders are not limited to the protection of specific states but extend to entire logical codespaces. In addition, we show that QNNs are able to discover new encoding rules, informed by the underlying noise, and we also discuss some of the main challenges and progress towards realistic experimental implementations in NISQ architectures.

Reinforcement learning for designing an atom interferometer

Liang-Ying Chih

JILA, University of Colorado Boulder

Contributing Speaker #4

We design an interferometer to measure acceleration in one dimension with high precision using ultracold atoms moving in an optical lattice. We utilize a branch of machine learning, reinforcement learning, to generate the shaking protocols needed to realize lattice-based analogs of elementary optical components, including a beam-splitter, a mirror, and a recombiner. The performance of these protocols is determined through fidelity measures that compare with ideal optical components. The interferometer's ability to measure acceleration is quantitatively evaluated using a Bayesian approach applied to measurements of the momentum distribution, and comparison is made with standard Bragg interferometers, demonstrating the potential for the application of reinforcement learning algorithms to these kinds of quantum sensing tasks.

Exploring Quantum Perceptron and Quantum Neural Network structures with a teacher-student scheme

Aikaterini Gratsea

ICFO - The Institute of Photonic Sciences, Castelldefels, Spain

Contributing Speaker #5

Near-term quantum devices can be used to build quantum machine learning models, such as quantum kernel methods and quantum neural networks (QNN) to perform classification tasks. There have been many proposals on how to use variational quantum circuits as quantum perceptrons or as QNNs. The aim of this work is to systematically compare different QNN architectures and to evaluate their relative expressive power with a teacher-student scheme. Specifically, the teacher model generates the datasets mapping random inputs to outputs which then have to be learned by the student models. This way, we avoid training on arbitrary data sets and allow us to compare the learning capacity of different models directly via the loss, the prediction map, the accuracy and the relative entropy between the prediction maps. We focus particularly on a quantum perceptron model inspired by the recent work of Tacchino et. al. [1] and compare it to the data re-uploading scheme that was originally introduced by Perez-Salinas et. al. [2]. We discuss alterations of the perceptron model and the formation of deep QNN to better understand the role of hidden units and non-linearities in these architectures.

[1] F. Tacchino, C. Macchiavello, D. Gerace, and D. Bajoni, npj Quantum Information 5 (2019), 10.1038/s41534-019-0140-4.

[2] A. Perez-Salinas, A. Cervera-Lierta, E. Gil-Fuster, and J. I. Latorre, Quantum 4, 226 (2020).

Scalable neural-network approach for learning quantum data directly from the physical model

Alexander Gresch

Quantum Technology Group, Heinrich-Heine-University

Contributing Speaker #6

The long-term goal of quantum computing is to solve critical problems a classical computer cannot accomplish efficiently. As this requires a fully-fledged quantum computer equipped with quantum error correction, it remains out of reach in the near future. In the mean time, considerable effort is spent on utilizing noisy intermediate scale quantum (NISQ) computers, most prominent hybrid classical-quantum algorithms, for approximately solving similar problems. However, these algorithms suffer from a daunting measurement effort and other challenges.
In this work, we take first steps towards a third possibility of exploiting a quantum computational advantage: We aim to combine classical machine learning and quantum data sets to solve problems that are out of reach for classical computers. Specifically, we develop a recurrent neural network set-up that can learn the quantum data by itself directly from the given physical model. The recurrent nature allows for the prediction of quantum data independent of its corresponding system size. This way, we bypass a crucial amount of data acquisition which has often proven a bottleneck for previous machine learning approaches. We showcase the set-up in the context of many-body localization (MBL). Unlike recent works on phase classification, we demonstrate that the preprocessed input data (such as the entanglement entropy) are themselves directly learnable from the system's Hamiltonian alone without any costly preprocessing step. Moreover, the flexibility in the system size enables the study of data extrapolated beyond the provided training set. In conjunction with a hybrid quantum algorithm providing trial quantum data, the extrapolation remains guidable even outside the classically reachable realm.

Optimized Observable Readout from Single-shot Images of Ultracold Atoms via Machine Learning

Axel Lode

University of Freiburg

Contributing Speaker #7

Single-shot images are the standard readout of experiments with ultracold atoms – the tarnished looking glass into their many-body physics. The efficient extraction of observables from single-shot images is thus crucial. Here, we demonstrate how artificial neural networks can optimize this extraction. In contrast to standard averaging approaches, machine learning allows both one- and two-particle densities to be accurately obtained from a drastically reduced number of single-shot images. Quantum fluctuations and correlations are directly harnessed to obtain physical observables for bosons in a tilted double-well potential at an unprecedented accuracy. Strikingly, machine learning also enables a reliable extraction of momentum-space observables from real-space single-shot images and vice versa. This machine-learning-based extraction requires only a single reconfiguration of the experimental setup between in-situ and time-of-flight imaging, thus potentially granting an outstanding reduction in resources.

Variational Learning for Quantum Artificial Neural Networks

Stefano Mangini

University of Pavia

Contributing Speaker #8

In the past few years, quantum computing and machine learning fostered rapid developments in their respective areas of application, introducing new perspectives on how information processing systems can be realized and programmed. The rapidly growing field of quantum machine learning aims at bringing together these two ongoing revolutions. Here, we first review a series of recent works describing the implementation of artificial neurons and feedforward neural networks on quantum processors. We then present an original realization of efficient individual quantum nodes based on variational unsampling protocols. We investigate different learning strategies involving global and local layerwise cost functions, and we assess their performances also in the presence of statistical measurement noise. While keeping full compatibility with the overall memory-efficient feedforward architecture, our constructions effectively reduce the quantum circuit depth required to determine the activation probability of single neurons upon input of the relevant data-encoding quantum states. This suggests a viable approach toward the use of quantum neural networks for pattern classification on near-term quantum hardware.

Neuromorphic Binarized Polariton Networks

Rafał Mirek

University of Warsaw, Faculty of Physics

Contributing Speaker #9

According to many economists, big data is the most important asset of the 21st century. The amount of generated information is exponentially growing. Finding an efficient and fast way of processing the data will have a huge impact on a future world. We propose a system performing neuromorphic computation using exciton-polaritons. They are quasiparticles obtained in a semiconductor microcavities as a result of strong coupling between photons and excitons. Polaritons are an excellent platform for information processing due to their small effective mass and strong nonlinearities. In our work we use nonlinear interactions present in nonequillibrium exciton-polariton Bose-Einstein condensate to create artificial neural network with efficiencies and speed beating top electronic systems in data classification problems.
The idea of implementing exciton-polariton system in neuromorphic networks is relatively new but it already led to successful realization of optical neural network performing reservoir computing [1,2]. We propose binarized network made of nonlinear XOR logic gates based on exciton-polariton condensate [3]. We perform classification of handwritten digits from MNIST dataset with 96 % accuracy in an opto-electronic realization of a binary network. We show all-optical XOR logic gate having outstanding energy efficiency (16 pJ per synaptic operation) and very high speed. Our work is the first step for building complex all-optical systems performing classification tasks with much better performance than previously observed.

[1] A. Opala, S. Ghosh, T. C. H. Liew, M. Matuszewski, Physical Review Applied 11, 064029 (2019).
[2] D. Ballarini, A. Gianfrate, R. Panico, A. Opala, S. Ghosh, L. Dominici, V. Ardizzone, M. De Giorgi, G. Lerario, G. Gigli, T. C. H. Liew, M. Matuszewski, and D. Sanvitto, Nano Letters 20, 3506 (2020).
[3] R. Mirek, A. Opala, P. Comaron, M. Furman, M. Król, K. Tyszka, B. Seredyński, D. Ballarini, D. Sanvitto, T. C. H. Liew, W. Pacuski, J. Suffczyński, J. Szczytko, M. Matuszewski, B. Piętka, Nano Letters 21, 3715-3720 (2021).

Quantum Camera

Iván Panadero Muñoz

Arquimea Research Center

Contributing Speaker #10

Quantum Metrology studies how to perform high-resolution and highly sensitive measurements of physical parameters using quantum mechanics to describe the interrogated system. Recently, quantum sensing has emerged as an unique and rapidly expanding field of study within quantum science and technology, with the most prevalent platforms being spin qubits, trapped ions, and flux qubits. In this work, we propose a measurement protocol based on neural networks for detecting inhomogeneous fields by interrogating an array of spin sensors. Further, a 2-qubit neural network will be designed using entanglement as a quantum resource to provide us with a higher resolution. Thus, we will navigate in an interplay of ideas both from machine learning and quantum computing, a field known as Quantum Machine Learning, with the goal of applying them in metrological tasks.

Scrambling Ability of Quantum Neural Network Architectures

Yadong Wu

Tsinghua University

Contributing Speaker #11

We propose a guiding principle for how to design the architecture of a quantum neural network in order to achieve a high learning efficiency. This principle is inspired by the equivalence between extracting information from the input state to the readout qubit and scrambling information from the readout qubit to input qubits. We characterize the quantum information scrambling by operator size growth. By Haar random averaging over operator sizes, we propose an averaged operator size to describe the information scrambling ability of a given quantum neural network architecture. The key conjecture of this work is that this quantity is positively correlated with the learning efficiency of this architecture. To support this conjecture, we consider several different architectures and we also consider two typical learning tasks. One is a regression task of a quantum problem and the other is a classification task on classical images. In both cases, we find that, for the architecture with a larger averaged operator size, the loss function decreases faster or the prediction accuracy increases faster as the training epoch increases, which means higher learning efficiency. Our results can be generalized to more complicated quantum versions of machine learning algorithms.

Chapter 2

Posters

Magic of the Restricted Boltzmann Machines

Arash Ahmadi

Delft University of Technology

Poster #1

One of the challenges in quantum many-body systems, is to find the ground state of a quantum system. Due to exponential growth in the scale of Hilbert space, it is not possible to numerically find the exact ground state. Recently, neural networks have proven to be flexible generic variational ansatze that help to approach this challenge. At the same time, the neural networks representations of quantum states are difficult to interpret. In this work, we approach the interpretability of neural network quantum states using tools from computational complexity theory and quantum information. Specifically, we show how to employ quantum computational complexity of these states as a measure of their approximative power.

Convolutional restricted Boltzmann machine aided Monte Carlo: An application to Ising and Kitaev models

Daniel Alcalde Puente

Forschungszentrum Jülich

Poster #2

Machine learning is becoming widely used in analyzing the thermodynamics of many-body condensed matter systems. Restricted Boltzmann machine (RBM) aided Monte Carlo simulations have sparked interest, as they manage to speed up classical Monte Carlo simulations. In the poster/talk, based on my paper (Phys. Rev. B 102, 195148), I will explain how we used the convolutional restricted Boltzmann machine (CRBM) method to reduce the number of parameters to be learned drastically by taking advantage of translation invariance. Furthermore, I will show that it is possible to train the CRBM at smaller lattice sizes, and apply it to larger lattice sizes. To demonstrate the efficiency of CRBM, I show the application to the Ising and honeycomb Kitaev models.

Efficient algorithm for arrhythmia detection using a linguistic approach

Nikita Andreev

National Research University Higher School of Economics

Poster #3

Atrial fibrillation is the most common type of arrhythmia, and this condition often precedes the onset of more severe clinical conditions like cerebral infarction. In this article we present new approach to arrhythmia detection which is based on the use of statistical features obtained from R-R intervals, as well as analysis of the variability of the heart rhythm by means of a special alphabet. This approach provides us with good performance with low computational cost.

Entanglement entropy on a fuzzy sphere using normalizing flows

Tomasz Andrzejewski

University of British Columbia

Poster #4

We apply machine learning techniques developed in [Han, Hartnoll 2017] to search for ground energy states of a real scalar field theory with a quartic interaction on a fuzzy sphere. We use variational quantum Monte Carlo with deep generative flows. We then compute entanglement entropy and mutual information of the fuzzy sphere states using two different factorizations of the Hilbert space.

Interpretable and unsupervised phase classification

Julian Arnold

University of Basel

Poster #5

Fully automated classification methods that yield direct physical insights into phase diagrams are of current interest. In particular, unsupervised methods do not require prior labelling or knowledge of the phases of matter to be characterized. Here, I present an unsupervised machine learning method for phase classification which is rendered interpretable via an analytical derivation of the functional relationship between its optimal predictions and the input data [1]. Given these findings, I propose and apply an alternative, physically-motivated, data-driven scheme which relies on the difference between mean input features. This mean-based method is not based on any predictive model and is thus computationally cheap and directly explainable, i.e., one has a complete understanding of why the method yields a given phase classification. As an example, I consider the physically rich ground-state phase diagram of the spinless Falicov-Kimball model for which popular unsupervised learning methods, such as principal component analysis (PCA) and k-means clustering, can be shown to fail.

[1] J. Arnold, F. Schäfer, M. Žonda, and A. U. J. Lode, arXiv:2010.04730 (2020).

Tracing non-Abelian anyons via impurity particles

ICFO - The Institute of Photonic Sciences, Castelldefels, Spain

Niccolò Baldelli

Poster #6

Non-Abelian excitations are an interesting feature of many fractional quantum Hall phases, including those phases described by the Moore-Read (or Pfaffian) wave function. However, the detection of the non-Abelian quasiparticles is challenging. Here, we consider a system described by the Moore-Read wave function, and assume that impurity particles bind to its quasiholes. Then, the angular momentum of the impurities provides a useful witness of the physics of the non-Abelian excitations. After writing down the many-body wave function describing both the Moore-Read liquid and the impurities, we determine the impurity angular momentum through Monte Carlo sampling, and we show that it suggests a quantum-statistical parameter =ab+P/2 for the quasiholes, where ranges from 0 for bosons to 1 for fermions. A reasonable agreement with the Monte Carlo results is obtained for a=1/4, b=1/8 and P=0,1 depending on the parity of the particle number in the Moore-Read liquid. This parity-dependence of the angular momentum serves as an unambiguous demonstration of the non-Abelian nature of the excitations.

Self-Organized Maps and Quantum State Classification

Ludmila Botelho

IITiS PAN

Poster #7

We proposed the application of unsupervised machine learning in the form of self-organizing maps for the purpose of analyzing the structure of the space of quantum states.
The geometry of quantum states remains an active field of research, especially in the context of higher-dimensional data. The structure of higher-dimensional quantum systems is not easy to visualize and the methods for projecting it on low-dimensional space is useful for tracing the execution of quantum algorithms. As such those methods could constitute an valuable addition to system supporting quantum programming development.

Determination of Vibrational Circular Dichroism spectra through a classical dynamic approach using polarisable force fields.

Jessica Bowles

ICP, Université Paris-Saclay

Poster #8

Vibrational circular dichroism (VCD) is the weak difference in absorption for chiral molecules between right- and left- polarized light in the infrared range. It has promising applications in pharmacology owing to its ability to determine absolute configurations of chiral molecules. The shape of VCD spectra is highly sensitive to minor changes in conformation and molecular interactions, which makes it a sensitive probe of conformational isomerism and solvation. [1]

Most approaches in VCD studies so far have rested on static [2] and dynamic DFT calculations. [3, 4] These calculations are computationally demanding and associated with short exploration times. We propose a classical molecular dynamics approach using the AMOEBA polarisable force field [5] to extend the exploration time with an accurate description of the electrostatic interactions. This method has been recently implemented in the Tinker software package [6] and takes into account anharmonic and temperature effects.

References:

[1] Christian Merten, Robert McDonald, and Yunjie Xu. Strong solvent-dependent preference of and stereoisomers of a tris (diamine) nickel (ii) complex revealed by vibrational circular dichroism spectroscopy. Inorganic chemistry, 53(6):3177–3182, 2014.
[2] Ariel Pérez-Mellor and Anne Zehnacker. Vibrational circular dichroism of a 2, 5-diketopiperazine (dkp) peptide: Evidence for dimer formation in cyclo ll or ld diphenylalanine in the solid state. Chirality, 29(2):89–96, 2017.
[3] Sascha Jähnigen, Arne Scherrer, Rodolphe Vuilleumier, and Daniel Sebastiani. Chiral crystal packing induces enhancement of vibrational circular dichroism. Angewandte Chemie International Edition, 57(40):13344–13348, 2018.
[4] Katia Le Barbu-Debus, Jessica Bowles, Sascha Jähnigen, Carine Clavaguéra, Florent Calvo, Rodolphe Vuilleumier, and Anne Zehnacker. Assessing cluster models of solvation for the description of vibrational circular dichroism spectra: synergy between static and dynamic approaches. Physical Chemistry Chemical Physics, 22(45):26047–26068, 2020.
[5] Jay W Ponder, Chuanjie Wu, Pengyu Ren, Vijay S Pande, John D Chodera, Michael J Schnieders, Imran Haque, David L Mobley, Daniel S Lambrecht, Robert A DiStasio Jr, et al. Current status of the amoeba polarizable force field. The journal of physical chemistry B, 114(8):2549–2564, 2010.
[6] J. W. Ponder. TINKER - Software Tools for Molecular Design (version 8). http://dasher.wustl.edu/tinker (accessed July 22th, 2020).

Improving the Training Efficiency of Gaussian Process Models of Potential Energy Surfaces via Boundary Optimisation

Jack Broad

University of Nottingham

Poster #9

A strategy is outlined to make the modelling of intermolecular potentials using Gaussian processes more computationally efficient. This is achieved by using an asymptotic function at long range, and by learning the cross-over distance between the Gaussian process and this function using the training data. This procedure, known as boundary optimisation, has produced promising results for a number of different implementations across various chemical systems, with results presented here for the HF-Ne potential. Boundary optimisation is undertaken using a direct search algorithm and achieves an improvement in training efficiency of up to $\tilde{4}5$ % for this system, compared with an equivalent method under which the cross-over distance is fixed. The versatility of a direct search is such that it is easily transferable to other statistical methods of prediction or modelling problems.

Unsupervised machine learning of topological phase transitions from experimental data

Niklas Käming

Universität Hamburg

Poster #10

Poster Recently, machine learning methods have been shown to be an alternative way of localizing phase boundaries also from noisy and imperfect data and without the knowledge of the order parameter. Using unsupervised machine learning techniques including anomaly detection and influence functions we obtain the topological phase diagram of the Haldane model in a completely unbiased fashion from experimental data. We show that the methods can successfully be applied to experimental data at finite temperature and to data of Floquet systems, when postprocessing the data to a single micromotion phase. Our work provides a benchmark for unsupervised detection of new exotic phases in complex many-body systems.

Inference of the potential from absorption images: Inverting density functional theory with ultracold atoms

Miriam Büttner

Institute of Physics, ALU Freiburg

Poster #11

We discuss an application of our new machine learning toolbox, the Universal Neural-Network Interface for Quantum Observable Readout from N-body wavefunctions (UNIQORN). We follow a strategy that is inverse to density functional theory: we infer the potential that a many-body system of indistinguishable bosonic particles is placed in from absorption or single-shot images, i.e., samples of the N-body state. We demonstrate the network's ability to correctly learn and generalize from such images in both real and momentum space. We thus open up new possibilities for the analysis of experimental single-shot images. The connection between the single-shot measurements and the inferred potential is investigated further in a comparison to potentials obtained via the Thomas Fermi (TF) approximation. The potentials inferred with our model are shown to be significantly more accurate than its TF counterparts. We plan to deploy our machine learning models for experimental data in the future.

A benchmark quantum chemistry study on CO2 clathrates: Exploring new data-driven interaction models

Adriana Cabrera

IFF-CSIC

Poster #12

Understanding of energetics and structural stability in inclusion compounds allows controlling properties involved in different industrial and technological applications like potential molecular materials in tackling important environment problems related to greenhouse gases capture and storage. We investigate guest-host/host-host interactions in clathrate hydrates, dominated by hydrogen bonds and van der Waals forces [1]. We focus on the evaluation of modern first-principles methodologies and the description of structural and dynamic processes in gas and condensed phases. We generate reference data from accurate quantum-mechanical calculations by testing different approaches on CO2 clathrates [2]. Such benchmark and systematic cross-check studies benefit new data-driven model research by providing high-quality training information, with new insights that indicate the underlying factors governing their structure-driven stability and triggering further investigations for controlling the stabilization of these promising long term CO2 storage materials [3].

Refrences:
[1] M. Goel, et al. CRC Press, 2019. A. Hassanpouryouzband, et al, Chem. Soc. Rev. 49(15), 5225-5309 (2020). A. Valdés, et al. J. Phys. Chem. C 119, 3945 (2015). D. J. Arismendi-Arrieta, et al. Chem. Eur. J. 24, 9353 (2018).
[2] A. Cabrera-Ramirez, et al. ChemPhysChem. 21, 2618 (2020). A. Cabrera-Ramirez, et al. ChemPhysChem. 22, 359 (2021). A. Cabrera-Ramirez, et al. J. Chem. Phys. 154, 044301 (2021).
[3] J. Behler, J. Chem. Phys. 145 (2016). T. Mueller, et al. J. Chem. Phys. 152 (2020).

Machine learning two bodies spin correlations

Francesco Carnazza

University of Tübingen

Poster #13

In recent years artificial Neural networks methods have established themselves as a sound tool to encode the state of both closed and open quantum systems. In the case of open quantum systems, we want to study the dynamics of two body correlations, and see if an (eventually time-local) generator can be extracted. The model considered is a spin chain where the system of interest is formed by two spin acting as an impurity coupled to a the bath consisting of the rest of the chain. The whole chain is evolved according to an experiment inspired Hamiltonian. From the reduced density matrix obtained tracing out the degrees of freedom of the environment, the two bodies correlations are obtained, which are subsequently used to train the network. A most simple architecture, multilayer perceptron, is adopted in order to have the possibility to "look inside" the network and compare it with the expected Lindblad dynamics.
The main goal of this research is thus to retrieve the form and the properties of the Lindblad superoperator.

Machine Learning Approach to Long Time Step Molecular Dynamics for Hard Sphere Systems

Ka Chun Chan

Karlsruhe Institute of Technology

Poster #14

Atomistic simulation techniques such as molecular dynamics (MD) provide an accurate and precise description of atomic motion, molecular structure and permit the prediction of the physical and chemical properties of molecular system. However, MD requires expensive computation of energy and force which leads to significant computational effort. This severely limits MD applications to biological system and soft matter physics on long time scales.

The usual MD time step is approximately 1/10 of the fastest frequency of the molecular system. In order to accelerate the MD computation, we propose a machine learning approach to propagate the molecular system instead of the usual MD time step. As a first step we developed a machine learning (ML) propagator for hard-sphere systems that propagates the molecular system with each atomic collision as a new time step. The proposed algorithm learns the time evolution of the atomic motion and the collision between atoms, such that the neural network are able to predict the system trajectory, identify the collided atomic pairs and correct the trajectory of the collided pairs for each collision time step. We will discuss the perspective of this newly ML propagator for the acceleration of MD simulations and further application to the molecular system with long time scales.

The Bayesian Committee Approach for Computational Physics Problems

Li Chen

Institute foradvanced study, Tsinghua University

Poster #15

We propose a method for efficient learning of a multi-dimensional function. This method combines the Bayesian neural networks and the query-by-committee method. A committee made of deep Bayesian neural networks not only can provide uncertainty of the prediction but also can provide the discrepancy between committee members. Both the uncertainty and the discrepancy are large in the regions where the target function varies rapidly, and therefore, both quantities can be used to guide sampling data to such regions. In this way, we can learn a function accurately with the number of queried data points much less than uniform sampling. Here we test our method with two examples. One example is to find a rare phase in a phase diagram, which is separated from other phases by a second-order phase transition. In this example, the target function is the susceptibility function, and since the divergence of the susceptibility function locates the phase diagram, the task of searching such a phase perfectly matches the advantage of our method. Another example is to learn the distribution function for Monte Carlo integration of a high-dimensional function. In both examples, we show that the performance of our method performs is significantly better than uniform sampling. Our method can find broad applications in computational scientific problems.

Interpretable machine learning and topological insulators

Zofia Cieślińska

University of Warsaw

Poster #16

The project aims to differentiate between two distinct insulating phases in the model of one dimensional topological insulator (Su-Schrieffer-Heeger model). In this task we use a neural network to choose whether a system is a topological or a classical insulator, basing on its eigenvectors. Although the problem is trivial in a basic, idealized version, it becomes a challenge for a neural network when some noise is introduced in the Hamiltonian. A custom convolutional neural network was used to solve the problem, along with an interpretable machine learning technique (class activation mapping - CAM) which was applied to confirm that the network learned from physical properties of the system, not from artifacts generated by the noise.

Deep learning methods for the computation of vibrational wavefunctions

Laia Domingo Colomer

Instituto de Ciencias Matemáticas (ICMAT)

Poster #17

In this work, two Deep Learning models are used to generate the ground and excited wavefunctions of different Hamiltonians suitable for the study of the vibrations of molecular systems. The generated neural networks are trained with Hamiltonians that have analytical solutions. Then the network is asked to generalize these solutions to more complex Hamiltonian functions. This approach allows the reproduction of the excited vibrational wavefunctions of different molecular potentials. All methodologies used here are data-driven, therefore they do not assume any information about the underlying physical model of the system. This makes this approach versatile, and can be used in the study of multiple systems in quantum chemistry.

An ansatz-agnostic method for the dynamics of low-entropy open quantum systems using neural networks

Kaelan Donatella

Univetsité de Paris

Poster #18

We propose a general numerical method for low entropy open quantum systems based on neural network ansätze. This is possible by extending our previous work [1] that consists in judiciously compressing a "corner" of the Hilbert space that faithfully represents the density matrix of a physical system, which contains M wavefunctions, with M of the order of the system size. By using variational ansätze for the wavefunctions that belong to this subspace, we propose a method that works independently of the chosen ansätze for the wavefunctions, and the time evolution of the subspace corresponds to the dynamics of a M closed systems. This work therefore enables one to use known techniques for closed systems (for instance, schemes using deep convolutional networks [2]) without relying on the purification ansatz that restricts the approach to restricted Boltzmann machines (RBMs) [3-6].

[1] K. Donatella, Z. Denis, A. Le Boité, C. Ciuti, Continuous-time dynamics and error scaling of noisy highly-entangling quantum circuits, arXiv 2021.
[2] M. Schmitt, M. Heyl, Quantum many-body dynamics in two dimensions with artificial neural networks, PRL 2020.
[3] M.J. Hartmann, G. Carleo, Neural-network approach to dissipative quantum many-body dynamics, PRL 2019.
[4] F. Vicentini, A. Biella, N. Renault, C. Ciuti, Variational neural-network ansatz for steady states in open quantum systems, PRL 2019.
[5] A. Nagy, V. Savona, Variational quantum Monte Carlo method with a neural-network ansatz for open quantum systems, PRL 2019.
[6] N. Yoshioka, R. Hamazaki, Constructing neural stationary states for open quantum many-body systems, PRB 2019.

A simple and versatile detection technique for cold atoms

Ioannis Drougkakis

IESL-FORTH

Poster #19

Ultracold atoms have demonstrated great prospects for both technological and fundamental science applications. In order to fully exploit their potential, a precise control of the atomic cloud that can manipulate the quantum features and harness quantum resources is required.
We report a robust method for measurement and control of the atom number in an ultracold atomic ensemble. The measurement is based on the Faraday paramagnetic effect: off-resonant light, when traveling through a polarized atomic cloud, experiences optical rotation at an angle that is proportional to the number of atoms. The proposed measurement does not destroy quantum coherences and has an insignificant effect on the atomic temperature, so that it can be used to perform quantum-enhanced measurements and prepare the atomic state at the start of an interferometer sequence. Control of the atom number is realized by the unavoidable atom-loss that is introduced by the measurement, since even far off-resonant light has a non-zero probability for absorption. This atom-loss mechanism will be employed to shrink an initial ensemble to the targeted size. With the proposed method, for the first time the quantum back-action of the measurement probe is exploited to improve the stability of the experiment.
Measuring with subatom- shot noise resolution will lead to number squeezed states of Bose Einstein Condensates and will pave the way for squeezing and entanglement generation for spectroscopy and interferometry.
Preliminary results with a smaller than 1% precision in controling the atom number has been achieved using this method and will be presented. Applications of the proposed research include atomic clocks, inertial sensors, quantum computing, quantum simulations and fundamental physics experiments such as gravitational detectors.

Anomaly Detection for Quantum Many Body Physics

Korbinian Kottmann

ICFO - The Institute of Photonic Sciences, Castelldefels, Spain

Poster #20

I will present our work on using anomaly detection with simulated data from matrix product states (MPS) and projected entangled pair states (PEPS) as well as experimental data, to map out phase diagrams of many body systems.
"Unsupervised phase discovery with deep anomaly detection"
arXiv:2003.09905
"Unsupervised machine learning of topological phase transitions from experimental data"
arXiv:2101.05712
Further tba

Fast Squeezing, Delta-Kick Cooling and Optimal control

Léonce Dupays

Université du Luxembourg

Poster #21

Fast control of quantum states finds applications in quantum information. It can be used to fight against decoherence or to increase the rate of information processing. Within this scope, we present new methods for the fast control of quantum states, notably in trapped-ions. We first present a reverse-engineering method to achieve fast squeezing [1], this method is generic and can be applied to different experimental platforms. We then find an exact formula to describe the Delta-kick cooling kick time [2], and demonstrate that the delta-kick cooling can be considered as a time-optimal process that is the limit of protocols known as "Bang-Bang" processes [4].

[1] L.Dupays, A. Chenu, Shortcuts to Squeezed thermal states, Quantum, 2021.
[2] L. Dupays, D.C Spierings, A.M Steinberg, A. del Campo, ArXiv:2104.00999.
[3] H. Ammann, N. Christensen, Delta Kick Cooling: A New Method for Cooling Atoms, PRL.
[4] T. Y. Huang, B.A. Malomed, X. Chen, Shortcuts to adiabaticity for an interacting Bose–Einstein condensate via exact solutions of the generalized Ermakov equation

Topological quantum critical points in extended Bose-Hubbard models

Joana Fraxanet Morales

ICFO - The Institute of Photonic Sciences, Castelldefels, Spain

Poster #22

Topological phases in quantum systems are usually characterized by a specific robust gap in the bulk and gapless edge states. When at critical points, the gap should vanish and therefore it is natural to believe that also the topological properties of the system are lost. Nevertheless, it has been recently demonstrated that for specific S=1 chains hosting the celebrated Haldane phase, a new topological regime may occur exactly at a quantum critical point. Here we show that these intriguing new topological states can also appear in extended Hubbard models and can therefore be experimentally investigated using ultracold magnetic atoms. Moreover, we demonstrate that such states appear also at phase transitions separating topological phases other than the Haldane phase, establishing topological quantum critical points as a rather general phenomena.

Studying disulfide shuffling with the aid of Machine Learning

Claudia Leticia Gomez Flores

Karlsruhe Institute of Technology

Poster #23

Due its computational efficiency, DFTB has positioned itself as a reliable quantum mechanical method for condensed phase applications, especially where an extensive sampling of the configurational space is important to the reactive process of interest such as chemical reactions in biological systems. However as a "low-method" can neglect certain energy contributions, or show inaccurate transition states, as seen in thiol-disulfide exchange, our system of interest. To learn and correct these DFTB miscalculations was the motivation of our project. To achieve this, a Behler–Parrinello-type Neural Network learnt the energy value differences between the ab initio quantum chemical potential and DFTB for a given molecular structure. The implementation of the machine learning correction into DFTB+ corrected the DFTB energy into Coupled Cluster level, the "gold standard" of quantum chemistry. Implementation of force calculation allowed to perform quantum mechanical simulations with the scaling of semi-empirical methods.

Convolutional Neural Networks for Long Time Dissipative Quantum Dynamics

Luis Eduardo Herrera Rodríguez

Universidad Nacional de Colombia

Poster #24

Exact numerical simulations of dynamics of open quantum systems often require immense computational resources. We demonstrate that a deep artificial neural network composed of convolutional layers is a powerful tool for predicting long-time dynamics of open quantum systems provided the preceding short-time evolution of a system is known. The neural network model developed in this work simulates long-time dynamics efficiently and accurately across different dynamical regimes from weakly damped coherent motion to incoherent relaxation. The model was trained on a data set relevant to photosynthetic excitation energy transfer and can be deployed to study long-lasting quantum coherence phenomena observed in light-harvesting complexes. Furthermore, our model performs well for the initial conditions different than those used in the training. Our approach reduces the required computational resources for long-time simulations and holds the promise for becoming a valuable tool in the study of open quantum systems.

Enhancing temperature corrections in open system quantum dynamics simulations with fully differentiable machine learning

Yannick Holtkamp

Jacobs University Bremen

Poster #25

Exact quantum dynamic calculations in open systems are important to understand many processes, such as the energy and charge transfer on surfaces of artificial light-harvesting systems. These calculations are often done using density matrix calculations, which however get too expensive for large system sizes. Alternatively, one can use a version of semi-classical Ehrenfest calculations called Numerical Integrations of Schrödinger Equation (NISE). The NISE however acts in the high-temperature limit and therefore does not reproduce the correct thermal distribution. Hence, some hand-crafted ad-hoc correction factors have been developed to get correct distributions. Here, I will present a new approach by implementing the NISE as a fully differentiable method and training a machine-learning algorithm to find a replacement for the hand-crafted correction based on exact density matrix calculations.
I will demonstrate that the results with the machine-learned correction factor produce significantly improved results compared to previous corrections especially in low system bath coupling regions that are of most interest for the NISE calculations.
The results open new possibilities and enable simulations with significantly more accurate results in systems where accurate density matrix calculations are too slow or otherwise not suitable. This could help to understand phenomena that require accurate dynamics in large systems.

Gutzwiller projected trial-states for quantum magnets at finite temperature

Friederike Horn

Ludwig-Maximilians - Universität München

Poster #26

Quantum gas microscopy can achieve single-site and spin-resolved detection of ultracold atoms in optical lattices. Being able to create such snapshots from a Hamiltonian provides an important link between theory and experiment. Here we propose a variational Monte Carlo method to sample the ground state of the 1D and 2D antiferromagnetic Heisenberg Hamiltonian at finite temperature. We construct a Gutzwiller projected density matrix from the eigenstates of a fermionic mean field approximation of the Heisenberg Hamiltonian. This enables us to compute the expectation value of the energy and approximate the entropy as a function of the mean fields and effective coupling constant. Minimizing the free energy we can thus obtain a variational ground state. We will present results in one and two-dimensional systems.

Approximate fermion many-body wave function by a feed-forward neural network

Koji Inui

Department of Applied Physics, The University of Tokyo

Poster #27

Recent developments in machine learning have a profound impact on the field of physics. In particular, neural network, which in principle can approximate any function, has been intensively studied as a new method to represent quantum many-body wave functions. So far, various methods have been proposed, such as the restricted Boltzmann machine [1,2], the convolutional neural network [3], and the Gaussian process approximation [4]. However, it is difficult to precisely approximate the complicated sign structure in many-body wave functions for fermionic systems and frustrated spin systems [5,6]. To avoid the difficulty, most previous studies for these systems combine the neural network ansatz with the wave functions based on the Slater determinant [2,3,7]. However, the calculation of the determinant is computationally costly, which scales to N^3 with the number of electrons N. In this study, we develop a method to approximate fermionic many-body wave functions by a neural network without using the Slater determinant. We implement two fully-connected neural networks for the particle configuration and an extended Gutzwiller-Jastrow approach. In addition, we make a modification to the Monte Carlo method for better stability of the calculation. We demonstrate the efficiency of our method for the Hubbard model in two dimensions.

[1] G. Carleo and M. Troyer, Science 355, 602 (2017). [2] Y. Nomura et al., Phys. Rev. B 96, 205152 (2017). [3] K. Choo, T. Neupert, and G. Carleo, Phys. Rev. B 100, 125124 (2019). [4] A. Glielmo et al., Phys. Rev. X 10, 041026 (2020). [5] T. Westerhout et al., Nat. Commun. 11, 1593 (2020). [6] A. Szabo and C. Castelnovo, Phys. Rev. Research 2, 033075 (2020). [7] J. Hermann, Z. Schätzle, and F. Noé, Nat. Chem. 12, 891 (2020).

Scalable Hamiltonian learning for large-scale out-of-equilibrium quantum dynamics

Guliuxin Jin

Delft University of Technology (TU Delft)

Poster #28

Large-scale quantum devices provide insights beyond the reach of classical simulations. However, for a reliable and verifiable quantum simulation, the building blocks of the quantum device require exquisite benchmarking. This benchmarking of large scale dynamical quantum systems represents a major challenge due to lack of efficient tools for their simulation. Here, we present a scalable algorithm based on neural networks for Hamiltonian tomography in out-of-equilibrium quantum systems. We illustrate our approach using a model for a forefront quantum simulation platform: ultracold atoms in optical lattices. Specifically, we show that our algorithm is able to reconstruct the Hamiltonian of an arbitrary sized bosonic ladder system using an accessible amount of experimental measurements. We are able to significantly increase the previously known parameter precision.

Application of accurate molecular spectra for studying molecular collisions and interactions

Hubert Jóźwiak

Nicolaus Copernicus University in Toruń

Poster #29

Accurate measurements of the shapes of molecular resonances provide information about molecular dynamics and validate the potential energy surfaces for various collisional systems. This is due to the fact that the collision-perturbed velocity distribution of the optical coherence manifests itself as the perturbation of the shape of such resonance. I will present a theoretical description of this process, using state-of-the-art potential energy surfaces and quantum scattering calculations for diatom-atom and diatom-diatom systems. Not only does this approach properly describe the internal and translational motions of the molecules, but also correlations between them. This results in the subpercent agreement between the calculated and measured spectral line profiles. These theoretical developments are important for reducing systematic errors in optical metrology based on molecular spectroscopy (for instance, they allow for more accurate determination of rovibrational splitting in molecular hydrogen and, hence, for accurate tests of quantum electrodynamics for molecules). Accurate theoretical models of the collision-perturbed molecular spectra will be used for populating line-by-line spectroscopic databases and providing reference spectra for the studies of planetary atmospheres.

Neural network enhanced hybrid quantum many-body dynamical distributions

Rouven Koch

Aalto University

Poster #30

Computing dynamical distributions in quantum many-body systems represents one of the paradigmatic open problems in theoretical condensed matter physics. Despite the existence of different techniques both in real-time and frequency space, computational limitations often dramatically constrain the physical regimes in which quantum many-body dynamics can be efficiently solved. Here we show that the combination of machine learning methods and complementary many-body tensor network techniques substantially decreases the computational cost of quantum many-body dynamics. We demonstrate that combining kernel polynomial techniques and real-time evolution, together with deep neural networks, allows us to compute dynamical quantities faithfully. Focusing on many-body dynamical distributions, we show that this hybrid neural-network many-body algorithm, trained with single-particle data only, can efficiently extrapolate dynamics for many-body systems without prior knowledge. Importantly, this algorithm is shown to be substantially resilient to numerical noise, a feature of major importance when using this algorithm together with noisy many-body methods. Ultimately, our results provide a starting point towards neural-network powered algorithms to support a variety of quantum many-body dynamical methods, that could potentially solve computationally expensive many-body systems in a more efficient manner.

London Dispersion Forces using a Variational Approach Without Density Distortion: From Wavefunction Ansatz to Molecular Benchmarking

Derk Kooi

Vrije Universiteit Amsterdam

Poster #31

Calculating intermolecular (van der Waals) forces is a challenging aspect of quantum chemistry, but extremely important for its use in chemistry and biology. Density Functional Theory (DFT), the workhorse of quantum chemistry, naturally captures the electrostatic and induction components of intermolecular forces, but has difficulty describing dispersion. The difficulty can be easily rationalized, since electrostatics and induction result from the electron density and distortion thereof, respectively, while dispersion is in fact a feature of the intermolecular electron pair density. This is remedied in practice by including empirical corrections based on the positions of nuclei and free atomic polarizabilities,[1,2] which suffer from deficiencies, such as lacking anisotropy and not allowing for a self-consistent correction of the density. In our work we have introduced a new class of wavefunctions, which allow for correlation of the electrons without electron density distortion.[3] This results in computational simplification and is conceptually appealing in the context of DFT. The resulting Fixed Diagonal Matrices (FDM) method[3-5] performs satisfactorily for closed-shell atoms and molecules when used with accurate (CCSD) pair densities, producing a Mean Average Percentage Error (MAPE) and Max Absolute Error (AMAX) of 7.1% and 18.2% for isotropic dispersion coefficients C6, respectively.[5] The method performs as well for anisotropic dispersion coefficients and can in principle be incorporated self-consistently.[4]

References

[1] Stefan Grimme, Andreas Hansen, Jan Gerit Brandenburg, and Christoph Bannwarth. Dispersion-corrected mean-field electronic structure methods. Chemical Reviews, 116(9):5105–5154, apr 2016. doi: 10.1021/acs.chemrev.5b00533. URL https://doi.org/10.1021%2Facs.chemrev.5b00533.

[2] Martin Stöhr, Troy Van Voorhis, and Alexandre Tkatchenko. Theory and practice of modeling van der waals interactions in electronic-structure calculations. Chemical Society Reviews, 48(15):4118–4154, 2019. doi: 10.1039/c9cs00060g. URL https://doi.org/10.1039%2Fc9cs00060g.

[3] Derk P. Kooi and Paola Gori-Giorgi. A variational approach to london dispersion interactions without density distortion. The Journal of Physical Chemistry Letters, 10(7):1537–1541, mar 2019. doi: 10.1021/acs.jpclett.9b00469. URL https://doi.org/10.1021%2Facs.jpclett.9b00469.

[4] Derk P. Kooi and Paola Gori-Giorgi. London dispersion forces without density distortion: a path to first principles inclusion in density functional theory. Faraday Discussions, 224:145–165, 2020. doi: 10.1039/d0fd00056f. URL https://doi.org/10.1039%2Fd0fd00056f.

[5] Derk P. Kooi, Timo Weckman, and Paola Gori-Giorgi. Dispersion without many-body density distortion: Assessment on atoms and small molecules. Journal of Chemical Theory and Computation, mar 2021. doi: 10.1021/acs.jctc.1c00102. URL https://doi.org/10.1021%2Facs.jctc.1c00102.

Quantum chaos in Feshbach resonances of the ErYb system

Maciej Kosicki

Institute of Physics, Kazimierz Wielki University, Bydgoszcz

Poster #32

We investigate ultracold magnetic-field-assisted collisions in the so far unexplored ErYb system. The nonsphericity of the Er atom leads to weakly anisotropic interactions that provide the mechanism for Feshbach resonances to emerge. The resonances are moderately sparsely distributed with a density between 0.1 G^{-1} and 0.3 G^{-1} and exhibit chaotic statistics characterized by a Brody parameter between 0.5 and 0.7. The chaotic behaviour of Feshbach resonances is accompanied by strong mixing of magnetic and rotational quantum numbers in near-threshold bound states. We predict the existence of broad resonances at fields < 300 G that may be useful for the precise control of scattering properties and magnetoassociation of ErYb molecules. The high number of bosonic Er-Yb isotopic combinations gives many opportunities for mass scaling of interactions. Uniquely, two isotopic combinations have nearly identical reduced masses (differing by less than 10^5 relative) that we expect to have strikingly similar Feshbach resonance spectra, which would make it possible to experimentally measure their sensitivity to hypothetical variations of proton-to-electron mass ratio.

Deep Learning of Quantum Entanglement

Dominik Koutny

Palacky University Olomouc

Poster #33

Quantum entanglement lies at the heart of quantum mechanics and quantum information processing. Phase transitions and topological states in condensed matter physics emerge as results of strong quantum correlations. Future quantum computers outperforming classical ones, i.e. reaching the quantum advantage, heavily relies on quantum entanglement as a resource. Advanced secure communication protocols of quantum cryptography also require quantum entanglement when the independence of the hardware layer is essential. Consequently, accurate quantification of an amount of entanglement in a physical system is of paramount importance to fundamental research and many cutting-edge applications. Various approaches to entanglement detection have been proposed. Still, they usually provide only a witness or a lower bound [1] or require the interference of multiple copies of the system under test [2], which is extremely challenging. It was shown that quantum tomography is necessary for the exact determination of entanglement in an unknown quantum state [3].

We focus on $1/2$ spin ensembles and photonic qubit sources composed of two-level subsystems and apply deep learning techniques to entanglement quantification. We estimate the entanglement measures, particularly the mutual information and concurrence [4], for two-qubit states using deep neural networks. These act on data from informationally incomplete measurements. We also provide a deep neural network with the measurement device description. In this way, the trained network can accept data from various measurement scenarios and perform, to some extent, independently of the measurement device. Furthermore, we generalize the neural network estimators to higher-dimensional systems. Our approach to entanglement 'learning' is more accurate and orders of magnitude faster than the state-of-the-art regularized maximum likelihood method. The presented results open the way for characterizing quantum sources on platforms, where collecting data for full tomography is highly resource demanding.

[1] H. Wunderlich, M. B. Plenio, Quantitative verification of entanglement and fidelities from incomplete measurement data, J. Mod. Opt. 56, 2100 (2009).
[2] R. Islam, et al. Measuring entanglement entropy in a quantum many-body system, Nature 528, 77 (2015).
[3] D. Lu, et. al., Tomography is necessary for universal entanglement detection with single-copy observables, Phys. Rev. Lett. 116 (2016).
[4] R. Horodecki, et al. Quantum entanglement, Rev. Mod. Phys. 81, 865 (2009).

Tensor networks and efficient descriptions of classical data

Ivan Kukuljan

Max Planck for Quantum Optics

Poster #34

We investigate the potential of tensor network based machine learning methods to scale to large image and text data sets. For that, we study how the mutual information between a subregion and its complement scales with the subsystem size L, similarly to how it is done in quantum many-body physics. We find that for text, the mutual information scales as a power law L with a close to volume law exponent, indicating that text cannot be efficiently described by 1D tensor networks. For images, the scaling is close to an area law, hinting at 2D tensor networks such as PEPS could have an adequate expressibility. For the numerical analysis, we introduce a mutual information estimator based on autoregressive networks, and we also use convolutional neural networks in a neural estimator method.

Deviations from Brownian motion

Gorka Muñoz Gil

ICFO - The Institute of Photonic Sciences, Cast elldefels, Spain

Poster #35

Deviations from Brownian motion leading to anomalous diffusion are ubiquitously found in transport dynamics, playing a crucial role in phenomena from quantum physics to life sciences. The detection and characterization of anomalous diffusion from the measurement of an individual trajectory are challenging tasks, which traditionally rely on calculating the mean squared displacement of the trajectory. However, this approach breaks down for cases of important practical interest, e.g., short or noisy trajectories, ensembles of heterogeneous trajectories, or non-ergodic processes. Recently, several new approaches have been proposed, mostly building on the ongoing machine-learning revolution. Aiming to perform an objective comparison of methods, we gathered the community and organized an open competition, the Anomalous Diffusion challenge (AnDi). Participating teams independently applied their own algorithms to a commonly-defined dataset including diverse conditions. Although no single method performed best across all scenarios, the results revealed clear differences between the various approaches, providing practical advice for users and a benchmark for developers.

Modeling and mitigation of realistic readout noise with applications to the Quantum Approximate Optimization Algorithm

Filip Maciejewski

Center for Theoretical Physics, Polish Academy of Sciences

Poster #36

Measurement noise is one of the main sources of errors in currently available quantum devices based on superconducting qubits. At the same time, the complexity of its characterization and mitigation often exhibits exponential scaling with the system size. In this work, we introduce a correlated measurement noise model that can be efficiently described and characterized, and which admits effective noise-mitigation on the level of marginal probability distributions. Noise mitigation can be performed up to some error for which we derive upper bounds. Characterization of the model is done efficiently using a generalization of the recently introduced Quantum Overlapping Tomography. We perform experiments on 15 (23) qubits using IBM's (Rigetti's) devices to test both the noise model and the error-mitigation scheme, and obtain an average reduction of errors by a factor >22 (>5.5) compared to no mitigation. Interestingly, we find that correlations in the measurement noise do not correspond to the physical layout of the device. Furthermore, we study numerically the effects of readout noise on the performance of the Quantum Approximate Optimization Algorithm (QAOA). We observe in simulations that for numerous objective Hamiltonians, including random MAX-2-SAT instances and the Sherrington-Kirkpatrick model, the noise-mitigation improves the quality of the optimization. Finally, we provide arguments why in the course of QAOA optimization the estimates of the local energy (or cost) terms often behave like uncorrelated variables, which greatly reduces sampling complexity of the energy estimation compared to the pessimistic error analysis. We also show that similar effects are expected for Haar-random quantum states and states generated by shallow-depth random circuits.

Development of a Classification Model for the Identification of Targets to Known P.aeruginosa Biofilm Formation Inhibitors

Rita Magalhães

FMUP-BioSIM@UCIBIO/REQUIMTE

Poster #37

Biofilms are syntrophic communities of microorganisms enclosed in a self-produced matrix and generally attached to a surface. Their formation confers high resistance to known antibiotics and natural host immune responses. Biofilm formation is complex and involves several mechanisms. P. aeruginosa is a highly pathogenic and resistant bacteria, responsible for up to 20% of hospital bacterial infections. Its capacity to form biofilms contributes to its high drug resistance. Several biofilm-formation P. a related protein targets have been identified, mainly involved in Quorum-Sensing, the cell-to-cell communication in bacteria, and motility. In the last few years, many ligands with biofilm formation inhibitory activity have been identified and experimentally tested. However, for many of these ligands, the specific molecular targets are unknown. Adequate knowledge of each ligand-target pair would allow for directed drug design and development, increasing chances of more potent inhibition.

In this work, a classification algorithm for the pairing of inhibitory ligands and protein targets in P.aeruginosa biofilm formation mechanisms was developed. Using Orange software (https://orangedatamining.com/), an implementation of machine learning train models was created using chemical descriptors extracted from a previously curated P. aeruginosa database. Classification models were tested, including logistic regression, support vector machines, decision trees, random forests, and neural networks. Models were trained and evaluated in the Python programming language, using the scikit-learn libraries. The algorithm was trained, validated, and tested with a set of known ligand-target pairs and can then be used to predict likely targets for newly discovered and developed inhibitors.

Deep learning based quantum vortex detection in atomic Bose-Einstein condensates

Friederike Metz

Okinawa Institute of Science and Technology

Poster #38

Quantum vortices naturally emerge in rotating Bose-Einstein condensates (BECs) and, similarly to their classical counterparts, allow the study of a range of interesting out-of-equilibrium phenomena like turbulence and chaos. However, the study of such phenomena requires to determine the precise location of each vortex within a BEC, which becomes challenging when either only the condensate density is available or sources of noise are present, as is typically the case in experimental settings. Here, we introduce a machine learning based vortex detector motivated by state-of-the-art object detection methods that can accurately locate vortices in simulated BEC density images. Our model allows for robust and real-time detection in noisy and non-equilibrium configurations. Furthermore, the network can distinguish between vortices and anti-vortices if the condensate phase profile is also available. We anticipate that our vortex detector will be advantageous both for experimental and theoretical studies of the static and dynamical properties of vortex configurations in BECs.

Approximating Excited States using Neural Networks

Yimeng Min

Cornell University

Poster #39

We propose a neural network method to solve the eigenstate problem in quantum mechanics. We combine the variational principle with a neural network wave function ansatz. Our method can approximate both the ground state and excited states. The approximation of excited states is realized by adding orthogonal constraints to energy expectation. We discuss both one-dimensional and two-dimensional conditions and the results are in good agreement with theoretical values. Our results demonstrate that the excited states can be approximated accurately by directly optimizing the parameters in a neural network.

Estimation of Thermodynamic Observables in Lattice Field Theories with Deep Generative Models

Kim Nicoli

Technische Universität Berlin

Poster #40

In our work we demonstrate that applying deep generative machine learning models for lattice field theory is a promising route for solving problems where Markov chain Monte Carlo (MCMC) methods are problematic. More specifically, we show that generative models can be used to estimate the absolute value of the free energy, which is in contrast to existing MCMC-based methods, which are limited to only estimate free energy differences. We demonstrate the effectiveness of the proposed method for two-dimensional 4 theory and compare it to MCMC-based methods in detailed numerical experiments.

Improving Machine Learning Models with Monotonicity Constraints

Anna Nikolaeva

Skolkovo Institute of Science and Technology

Poster #41

There is a huge need for interpretable machine learning models for tabular data. In particular, it is vital to construct neural network models that are monotonic concerning specific input features. One of the recently proposed methods is multidimensional polynomial lattices. The advantage of this model is that it has better prediction quality than the monotonous-constrained alternatives. However, the main disadvantage of constrained models is scalability. Thus, we consider techniques for clustering and ensembling these models to find the best trade-off between the quality of prediction and computational costs. In particular, we propose a method for constructing better ensembles of monotonic neural networks based on training diverse models. We evaluate the developed approaches on the synthetic data and open-source datasets.

A quantum algorithm for pattern matching

Pradeep Niroula

University of Maryland, College Park

Poster #42

Algorithms that search for a pattern within a larger data-set appear ubiquitously in text and image processing. Here, we present an explicit, circuit-level implementation of a quantum pattern-matching algorithm that matches a search string (pattern) of length M inside a longer text of length N. Our algorithm has a time complexity of $(\sqrt{N})$, while the space complexity remains modest at O(N+M). We report the quantum gate counts relevant for both pre-fault-tolerant and fault-tolerant regimes.

Machine learning classification of two-dimensional vortex configurations

Rama Sharma

Swinburne University of Technology, Australia

Poster #43

Non-equilibrium behavior of classical and quantum systems is ubiquitous in nature and includes interesting and complex phenomena such as turbulence. The quantum turbulence extends to the dynamics of superfluids such as Bose-Einstein condensates (BECs) and hence the topological excitations of quantized vortices within such systems can be considered as a key element to understand the problem of quantum turbulence. Thus, there is a need to identify the precise vortex phases of matter and phase transitions within a BEC. Identifying such transitions is one of the key challenges in quantum many-body problem. Recently, booming advancement in the field of machine learning procedures have been proven to be an alternative way to probe such problems effectively [1-4]. We introduce an unsupervised machine learning approach for classifying the vortex phases as a function of inverse temperature. We consider computer generated configurations of quantised vortices in planar superfluid Bose–Einstein condensates. We show that unsupervised machine learning technology can successfully be used for classifying vortex configurations to identify prominent vortex phases of matter from experimentally relevant data. The machine learning approach could be applied for automatically classifying large data sets of vortex configurations in experiments on two-dimensional quantum turbulence.

Waveguide adjustment using reinforcement learning

Robert Okuła

International Centre for Theory of Quantum Technologies, University of Gdańsk

Poster #44

We study the utilization of machine learning algorithms in the process of adjustment of misaligned wave-guides when the signal is described as Poisson process and in the environment with large shot noise ratio. Such scenario corresponds to aligning optical components of a single photon source. Using the reinforcement learning techniques, we construct and compare the results for two distinct first choice solutions for continuous action space: TD3 and SAC. Networks were subsequently trained on the simulated environment that was an appropriate simplification of the real-world environment. The results are compared based on the training process (average reward and episode lengths) as well as the success ratio

Feed-forward exciton-polariton neural network

Andrzej Opala

Institute of Physics, Polish Academy of Sciences

Poster #45

Technological solutions based on CMOS technology reach the physical limits imposed by quantum effects. Progress in computing and communication enforces the necessity to process large data sets in an ever shorter time. Unfortunately, the performance of commonly used computers based on the von Neumann architecture reaches its limit. This limitation results in the von Neumann bottleneck. Physical limits of the miniaturisation of integrated circuits make it impossible to solve this problem traditionally. Arguably, the best solution to avoid the technological impasse is using an optoelectronic system with architecture inspired by the structure of a brain. The features which are crucial for a so-called neuromorphic computing system are: the non-linearity of the active medium, the possibility of precise input state manipulation, scalability, energy efficiency and speed of operation. All of the above criteria are fulfilled by exciton-polariton quantum fluids of light [1,2,3]. This work demonstrates the first experimental realisation of a feed-forward exciton-polariton neural network optimised using a backpropagation algorithm. The backpropagation algorithm allows a significant improvement of neural network performance. The presented method enables effective applications of polariton networks that contain only several neurons.

[1] D. Ballarini, A. Gianfrate, R. Panico, A. Opala et all. Nano Lett, 20, 5, 3506–3512 (2020)
[2] R. Mirek, A. Opala, P. Comaron, M. Furman et all. Nano Lett. (2021)
[3] A. Opala, S. Ghosh, T. C. H. Liew and M. Matuszewski, "Neuromorphic computing in Ginzburg-Landau lattice systems", Phys. Rev. Applied 11, 064029, (2019)
[4] "Teaching a neural network with non-tunable exciton-polariton nodes" (in preparation)

On the quasiparticle nature of the Bose polaron at finite temperature

Gerard Pascual López

Universitat Politècnica de Catalunya

Poster #46

The Bose polaron has attracted theoretical and experimental interest because the mobile impurity is surrounded by a bath that undergoes a superfluid-to-normal phase transition. Although many theoretical works have studied this system in its ground state, only few analyze its behavior at finite temperature. We have studied the effect of temperature on a Bose polaron system performing ab-initio Path Integral Monte Carlo simulations. This method is able to approach the critical temperature without losing accuracy, in contrast with perturbative approximations. We have calculated the polaron energy for the repulsive and attractive branches and we have observed an asymmetric behavior between the two branches. When the potential is repulsive, the polaron energy decreases when the temperature increases, and contrariwise for the attractive branch. Our results for the effective mass and the dynamical structure factor of the polaron show unambiguously that its quasiparticle nature disappears close to the critical temperature, in agreement with recent experimental findings. Finally, we have also estimated the fraction of bosons in the condensate as well as the superfluid fraction, and we have concluded that the impurity hinders the condensation of the rest of bosons.

Qubits, topology and the SSH model

Nikolaos Petropoulos

University College Dublin

Poster #47

We firstly make a review of the 1D topological Su-Schrieffer-Heeger (SSH) model. We study the model with periodic and open boundary conditions (PBC and OBC) in different configurations, some of them breaking the chiral symmetry of the model and discuss the implications. Also, we demonstrate robustness to noise of the topological states and propose an idealized charge qubit design based on the model. Finally, we show a possible way to detect the presence of topological order in the system using equilibrium dynamics, utilizing the quantum informatic measure of mutual information I[b:e](t) as a measure of bulk-edge quantum correlations and offer a few remarks on possible future explorations.

Machine learning assisted identification of topological invariants in topological superconductors

Marcin Płodzień

MagTop Research Centre, Institute of Physics, Polish Academy of Sciences

Poster #48

One of the most significant challenges in the topological matter is the determination of global topological invariants from local measurements. Solving this problem will enable significant advances in the physics of topological materials. In particular, it could pave the way to experimentally determine the Chern number in two-dimensional chiral superconductors. We investigate the utilization of supervised machine learning to determine Chern numbers from the local density of states measurements in disordered Shiba lattice.

Quantum point spread function for imaging trapped few-body systems with a quantum gas microscope

Maxim Pyzh

Center for Optical Quantum Technologies (ZOQ), University of Hamburg

Poster #49

We propose a scheme to image the density distribution of a trapped few-body system with a high resoltion by ramping up a pinning lattice, freezing the atoms and detecting their positions by fluorescene imaging. A high resolution is reached by changing the relative position of the lattice. A subsequent averaging reveals a distortion of the original density distribution due to the non-adiabaticity of the ramping protocol, especially when the local structures of the density display variations on the scale of the pinning lattice spacing. We show that this dynamics can be described by a convolution filter, which we call in analogy to classical optics a quantum point spread function. Using a machine learning approach, we demonstrate via several experimentally relevant setups that a suitable deconvolution allows to partially recover the original density distribution.

netQuil

Matthew Radzihovsky

MIT

Poster #50

NetQuil is an open-source Python framework for quantum networking simulations built on the quantum computing framework pyQuil, by Rigetti Computing. NetQuil is built for testing ideas in quantum network topology and distributed quantum protocol. This platform allows users to create multi-agent networks, connect parties through classical and quantum channels, and introduce realistic noise and device models. NetQuil also makes running multiple trials for non-deterministic experiments, reviewing traffic in real-time, and syncronizing agents based on local and master clocks simple and easy. We provide an overview of the state of distributed quantum protocol, as well as a basic introduction to netQuil's framework. We present several demonstrations of canonical quantum information protocol built using netQuil's distributed quantum gates and pyQuil. We hope netQuil allows users to explore the quantum playground and the possibilities of distributed quantum computing.

Time-dependent variational principle for open quantum systems with artificial neural networks

Moritz Reh

Heidelberg university

Poster #51

We develop a variational approach to simulating the dynamics of open quantum many-body systems using deep autoregressive neural networks. The parameters of a compressed representation of a mixed quantum state are adapted dynamically according to the Lindbald master equation by employing a time-dependent variational principle. We illustrate our approach by solving the dissipative quantum Heisenberg model in one and two dimensions for up to 40 spins and by applying it to the simulation of confinement dynamics in the presence of dissipation.

Analyzing Neural Networks used for Classifying Snapshots of the Doped 1D t-J Model

Christian Reinmoser

University of Munich

Poster #52

Microscopic descriptions of quantum many-body systems are challenging, and even with approximate theoretical descriptions at hand it can be difficult to judge how well they perform. Hence, comparing snapshots of competing theoretical approaches with experimental data is a promising application for neural networks in quantum many-body physics. In a similar fashion, we implement simple network structures to classify three different classes of numerical data for the one-dimensional t-J model: DMRG as exact numerical approach and two Monte Carlo approaches. Specifically, we use a Gutzwiller projected mean-field approach and a squeezed space approach for the Monte Carlo sampling. We are able to find which Monte Carlo approach yields snapshots more similar to DMRG and which correlation functions yield classification results similar to the networks. In particular, we find that the squeezed space approach snapshots are more similar to the DMRG snapshots for large values of t/J and that two-point correlation function are significantly different between the snapshots of the two Monte Carlo classes to classify snapshots efficiently. The weights of the network suggest that the spin-spin and hole-hole correlation functions can be used for this specific classification task. With this approach we are able to use neural networks to establish which Monte Carlo approach approximates the DMRG data more accurately and we find two two-point correlation functions reproducing the classification of snapshots similar to the neural networks.

Classification of quantum phases with quantum machine learning

Juan Román-Roche

Institute of Nanoscience and Materials of Aragón (INMA), CSIC-University of Zaragoza

Poster #53

We show that a Support Vector Machine with a quantum kernel provides an accurate prediction of the phase transition in quantum many-body models, even when trained far from the critical point. The surging popularity of machine learning techniques has prompted their application to the study of physical properties, in particular to the detection of phase transitions. Recently, SVMs have been successfully employed for the prediction of the critical point of the 2D classical Ising model [1]. At the same time, machine learning has hybridized with quantum computation to yield quantum machine learning, where neural networks are replaced by variational quantum circuits and classical kernels give way to quantum kernels. These leverage the exponentially large Hilbert space in their favour, providing rich feature spaces where complex datasets can be accurately classified and promising a quantum advantage [2] [3]. However, many proposals ignore the challenge of loading classical data onto quantum memory or deal with synthetic data sets with no practical applications. In this context, we find that the study of quantum many-body systems provides the perfect testbed in the search for a practical quantum speed up, because the ground state wavefunctions that constitute the data set are quantum in origin, and thus classically intractable in large systems.
In this poster we train a SVM with a kernel constructed with numerically calculated ground states of the the Ising chain in transverse field (ICTF) at different extremes of the ferromagnetic constant J. The SVM learns to classify the two phases and is then able to correctly classify a set of ground states spanning uniformly along J, giving us an estimation of the critical point Jc. We then perform a finite size scaling analysis to extract the N $\rightarrow$ critical point. To benchmark our results, we replicate the results in [4] where a dip in the fidelity, the overlap between adjacent ground states in a uniform sampling of J, is used as a signature of the phase transition. We show that quantum-kernel SVMs, despite being trained with samples far from the phase transition, are an excellent tool to accurately predict quantum critical points.

[1] C. Giannetti, B. Lucini and D. Vadacchino, Nucl. Phys. B. 944, 114639 (2019)

[2] M. Schuld and N. Killoran, Phys. Rev. Lett. 122, 040504 (2019)

[3] Y. Liu, S. Arunachalam and K. Temme "A rigorous and robust quantum speed-up in supervised machine learning", arXiv:2010.02174v2 [quant-ph]

[4] SHI-JIAN GU, Int. J. Mod. Phys. B 24, 4371-4458 (2010)

Learning to measure: adaptive informationally complete POVMs for near-term quantum algorithms

Matteo Rossi

University of Helsinki

Poster #54

Variational quantum algorithms stand as the most promising approaches towards practical applications of near-term quantum computers. However, these methodologies usually require a large number of measurements, which represents an important roadblock for future real-world use cases. We introduce a novel approach to tackle this problem: a variational measurement scheme. We present an algorithm that optimises informationally complete POVMs on the fly in order to minimise the statistical fluctuations in the estimation of relevant cost functions. We use it in combination with the Variational Quantum Eigensolver to calculate ground-state energies of molecular Hamiltonians in numerical simulations and show that it is competitive with state-of-the-art measurement reduction approaches. We also highlight the potential of the informational completeness of the measurement outcomes by reusing the ground-state energy estimation data to perform high-fidelity reduced state tomography.

Extracting the positions of individual Si:P dopants from STM images

Piotr Różański

Nicolaus Copernicus University in Toruń

Poster #55

Atomic-scale solid-state qubits could be implemented using scanned-probe lithography to place two or more phosphorus dopants in silicon close to each other. Scanning tunnelling microscopy (STM) has been used to image individual dopants and to find dopant positions in the host silicon lattice based on that image. Determining the geometry of two-dopant qubits will be an essential step in device fabrication, however, double dopant-based devices will lead to a more challenging problem due to the complicated inter-valley wave-function interference patterns.

Here we propose a theoretical solution to that problem. We utilize a multi-million atom tight-binding method, accounting for d-orbitals, surface passivation and surface reconstruction. Further, we use a machine learning approach to determine the positions of both dopants based on STM images generated with tight-binding simulations. It is shown that even a simple neural network can learn to extract the dopants' positions with sufficient accuracy. Together with a possible calibration with experimental data, the proposed method forms a practical scheme for analysing multi-dopant experimental STM images.

Learning from the electron densities of atom types in Multipolar Atom Types from Theory and Statistical clustering (MATTS) databank

Paulina Rybicka

University of Warsaw Biological and Chemical Research Centre

Poster #56

Paulina Rybicka, Marta Kulik, Paulina Maria Dominiak

University of Warsaw, Warsaw, Poland
p.rybicka@uw.edu.pl

Keywords: multipole model, electron density, pseudoatoms databank, multidimensional clustering

Independent Atom Model (IAM) is the most widely used model in crystal structure refinement on X-ray or electron diffraction data. IAM assumes spherical symmetry of atomic densities, ignoring the charge redistribution due to chemical bonding. However, more accurate models of electron densities are available, such as the Multipole Model (MM). MM represents an aspherical approach and describes the surroundings of a nucleus far more accurately by using the Hansen-Coppens pseudoatom formalism [1]. In the MM, the electron density parameters of pseudoatoms appeared to be almost identical for atoms of one element located in a similar chemical environment. For that reason, banks of transferable aspherical atoms with universal parameters were created. MATTS (Multipolar Atom Types from Theory and Statistical Clustering) databank is one of them and supersedes previously used UBDB (University at Buffalo DataBank) [2]. It contains over 600 different atom types categorized by central element type and the topology of chemical surroundings, with information about the electron density distribution.

The main idea behind the project was to determine the relationships between electron densities of atom types and to organize the databank into reasonable groups. Clustering based on topology or density parameters was used for that purpose. The topology clustering took into account the information about the number and type of atoms' neighbors, local symmetry and planarity. It allowed visualizing the databank as a series of trees. For electron density clustering, the Density-Based Spatial Clustering of Applications with Noise (DBSCAN) method was used to do multidimensional clustering of all parameters. The results from topology and density clustering were compared searching for common features. Such analysis allowed to capture similarities in the spatial distribution of electron density for atom types, identify errors and also made it possible to categorize atom types into general and specific ones. Finally, it helped to understand which topology features influence the electron density the most.

Crystallographic databases, such as the Cambridge Structural Database (CSD), containing over a million small-molecule organic and metalloorganic crystal structures obtained mainly from X-ray and neutron diffraction methods, are sources of a variety of information about molecules. The CSD may provide new descriptors (like bond lengths or valence angles, for example) that can be used to better characterize atom types in the MATTS bank and to correlate with electron density descriptors. The whole variety of structural descriptors can further be used in both descriptive and predictive analysis of the MATTS databank using machine learning. The resulting algorithm will enhance the transferability of electron density parameters and allow the user to control the level of transferability error. It can provide the possibility for future users of MATTS to decide how many and how detailed atom types they prefer to use. That could be useful in refining structures, eliminating deficiencies of IAM. It may also serve as a fast tool to reconstruct the electron density of any (macro)molecule at a desired level of accuracy.

The authors acknowledge NCN UMO-2017/27/B/ST4/02721 grant.

References:

[1] Hansen, N. K., Coppens, P. (1978). Acta Cryst. A34, 909–921.

[2] Kumar, P., Gruza, B., Bojarowski, S. A.
Dominiak, P. M. (2019). Acta Cryst. A75, 398-408.

Spectral deep-learning for (ro-)vibrational calculations of weakly-bound molecules

Yahya Saleh

Center for Free-Electron Laser Science (CFEL) in Hamburg and Department of Mathematics, Universität Hamburg

Poster #57

Weakly-bound complexes are very appealing for experimental investigations of resonances in dissociation dynamics, which are of vital importance to roaming reactions [1,2]. Planning and elucidating experiments requires accurate quantum mechanical calculations of (ro-)vibrational energies up to dissociation, which is a challenging task for these systems because of their flexible degrees of freedom and large configuration space. Standard predictions for these problems represent the wavefunctions as a linear combination of some fixed basis set. The quality of the predictions highly depend on the choice of the basis set and the computational costs scale poorly with the dimension of the problem. Unlike linear variational methods, neural network-based models seem to scale relatively well with the dimension of the problem [3] and were successfully implemented to model ground-states of quantum systems [4,5,6]. However, extensions to excited states are still under-researched and are mostly performed in a sequential manner for low-lying exited states [7]. We present a nonlinear variational framework to simultaneously compute several eigenfunctions of linear operators acting on infinite-dimensional Hilbert spaces. The key principle is to treat neural networks as an adaptive basis set and use alternative optimisation, in a manner similar to [8].

Y. Saleh (1,2), Jannik Eggers (1,2), V. Sanjay (1,2,3), A. Iske (2), A. Yachmenev (1,3) , J. Küpper (1,3,4)

1- Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany

2- Department of Mathematics, Universität Hamburg, Hamburg, Germany

3- Center for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany

4- Department of Physics, Universität Hamburg, Hamburg, Germany

[1] M. Johny, J. Onvlee, T. Kierspel, H. Bieker, S. Trippel, J. Küpper, Chem. Phys. Lett. 721, 149 (2019).

[2] D. Townsend, S. A. Lahankar, S. K. Lee, S. D. Chambreau, A. G. Suits, X. Zhang, J. Rheinecker, L. B. Harding, J. M. Bowman, Science 306, 1158 (2004).

[3] E. Weinan and B. Yu, The deep ritz method: a deep learning-based numerical algorithm for solving variational problems, Commun. Math. Stat. 6, 1 (2018).

[4] G. Carleo and M. Troyer, Solving the quantum many-body problem with artificial neural networks, Science 355, 602 (2017).

[5] J. Hermann, Z. Schatzle, and F. Noe, Deep-neural-network solution of the electronic Schrödinger equation, Nat. Chem. 12, 891 (2020).

[6] D. Pfau, J. S. Spencer, A. G. Matthews, and W. M. C. Foulkes, Ab initio solution of the many-electron Schrödinger equation with deep neural networks, Phys. Rev. Research 2, 033429 (2020).

[7] K. Choo, G. Carleo, and N. Regnault, Symmetries and many-body excitations with neural-network quantum states, Phys. Rev. Lett. 121, 16 (2018).

[8] S. Manzhos, K. Yamashita, and T. Carrington Jr, Using a neural network based method to solve the vibrational Schrödinger equation for H2O, Chem. Phys. Lett. 474, 217 (2009).

DvD-TD3 Pytorch Implementation

Mariia Samsikova

ITMO University

Poster #58

One of the key challenges in Reinforcement Learning (RL) is the exploration-exploitation trade-off. Various methods can be used to acquire diverse experience. One possible method is to train a population of agents and use the distance between policies to stimulate their divergence. In " Effective diversity in population based reinforcement learning" paper, a novel method of measuring the distance between policies in the space of behavioural embeddings was proposed.To the best of my knowledge, I am the first one to implement the Twin Delayed Deep Deterministic Policy Gradient version of Diversity via Determinants(DvD-TD3) algorithm. Source code is publicly available at https://github.com/holounic/DvD-TD3.

Active learning of potential energy surfaces of weakly-bound molecular complexes

Vishnu Sanjay

DESY

Poster #59

Active learning of potential energy surfaces of weakly-bound molecular complexes

V. Sanjay(1,2,3), Y. Saleh(1,2), A. Iske(2), A. Yachmenev(1,3), J. Küpper(1,3,4)
(1) Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany
(2) Department of Mathematics, Universität Hamburg, Hamburg, Germany
(3) Center for Ultrafast Imaging, Universität Hamburg, Hamburg, Germany
(4) Department of Physics, Universität Hamburg, Hamburg, Germany

Weakly-bound complexes of organic molecules with water play diverse roles in various fields ranging from biology and chemistry to atmospheric science and astrochemistry. Accurate quantum mechanical computations of molecular dynamic in weakly-bound complexes are challenging because of the large-amplitude character of the intermolecular motions, resulting in a complex shape of the potential energy surface exhibiting multiple minima and saddle points [1]. The exponential scaling of the computational burden with the number of degrees of freedom, i.e., cluster size, renders the computational costs of existing variational methods unaffordable for clusters composed of more than two moieties.

We present a recent application of machine learning for simulations of the dynamics a weakly-bound dimer of pyrrole with water [2]. In particular, we present a new active learning algorithm designed for the construction of multi-dimensional ab initio potential energy surfaces using a minimum number of electronic structure calculations. The proposed algorithm is empirically shown to work better than the query-by-committee algorithm, a popular choice for building potential energy surfaces. Furthermore, the proposed method comes with a relatively small computational burden due to the use of regression trees.

[1] D. Townsend, S. A. Lahankar, S. K. Lee, S. D. Chambreau, A. G. Suits, X. Zhang, J. Rheinecker, L. B. Harding, J. M. Bowman, Science 306, 1158 (2004).
[2] Y. Saleh, V. Sanjay, A. Iske, A. Yachmenev, and J. Küpper, arXiv:2104.00708 [Physics] (2021).

Nonlocal kinetic energy functionals based on a Yukawa potential kernel

Fulvio Sarcinella

University of Salento - Istituto Italiano di Tecnologia

Poster #60

Density Functional Theory (DFT) has been, since long, one of the most employed tools to study electronic systems. In its original and most efficient formulation, namely Orbital-Free DFT (OF-DFT) [1], it requires reliable approximations for the noninteracting kinetic energy (KE) functional. This is not a straightforward task, because the KE is a major component of the total electronic energy and it is intrinsically nonlocal.
Over the years a great effort has been put in this topic resulting in the development of numerous KE functionals [2]. They can be divided into two main families: those costructed from local quantities (i.e. derivatives of the electronic density) and those based on a nonlocal kernel. Both have advantages and disadvantages, but none of the approaches can yield accurate and generally applicable functionals.
In this contribution I propose a new strategy for the development of KE functionals that join the main advantages of both the classes [3]. This makes use, together with local quantities, of a nonlocal ingredient based on the Yukawa potential. This approach allows to construct KE functionals (yGGA) of increased accuracy, especially for what concerns the linear response behavior, and of good general applicability.
As a proof of concept I have constructed a simple yGGA functional depending only linearly on the nonlocal ingredient. This has been succesfully tested on jellium spheres, considerning KE, potentials and the linear response.
Further work is in progress to develop yGGA functionals with a more complex functional dependence on the nonlocal ingredient.

[1] P. Hohenberg and W. Kohn, Inhomogeneous electron gas, Phys. Rev. 136, B864 (1964)

[2] L. A. Constantin, E. Fabiano and F. Della Sala, Performance of Semilocal Kinetic Energy Functionals for Orbital-Free Density Functional Theory, J. Chem. Theory Comput. 15, 3044 (2019)

[3] F. Sarcinella, E. Fabiano, L. A. Constantin and F. Della Sala, Nonlocal kinetic energy functionals in real space using a Yukawa-potential kernel: Properties, linear response, and model functionals, Phys. Rev. B 103, 155127 (2021)

Automatic Forest Inventory Using Satellite Imagery

Abduragim Shtanchaev

O.Vision

Poster #61

For many countries like Russia, Canada, or the USA, a robust and detailed tree species inventory is essential to manage their forests sustainably. Since one can not apply unmanned aerial vehicle (UAV) imagery-based approaches to large-scale forest inventory applications, the utilization of machine learning algorithms on satellite imagery is a rising research topic. Although satellite imagery quality is relatively low, additional spectral channels provide sufficient information for classification tasks. Assuming that tree crowns are detected already, we use embeddings of tree crowns generated by Autoencoders as a data set to train classical Machine Learning algorithms. We compare our Autoencoder (AE) based approach to traditional convolutional neural networks (CNN) end-to-end classifiers.

Quantized Bubble Nucleation

Aritra Sinha

Jagiellonian UniversityQuantized Bubble Nucleation

Poster #62

Non-equilibrium dynamics of slow quenches across continuous phase transitions have been understood very successfully under the unifying theory of the Kibble-Zurek mechanism. However, relatively little attention has been paid to understanding non-equilibrium dynamics across first-order quantum phase transitions (FOQPT). In an attempt to mitigate this, here I will show the consequences of a slow dynamical ramp across the FOQPT transition line present in the Ising model with both transverse and longitudinal fields [1]. The existence of a potential barrier, quintessential to the FOQPTs, gives rise to metastability in the dynamical state. Such metastability can wear off either by dynamical instability due to the disappearance of the potential barrier or by nucleating bubbles of the true vacuum driven by quantum fluctuations. While the former scenario has been studied across certain first-order phase transitions under the framework of Kibble-Zurek theory, here I will present our analysis of the generic situation of the breakdown of metastability by nucleation of bubbles. Specifically, we identify special resonant regions in the longitudinal field, where the metastable state can easily tunnel to nucleate bubbles of specific sizes, connected by perturbative processes (in the transverse field) of corresponding specific orders. Further, I will attempt to explain the entire non-adiabatic process under the umbrella of Landau- Zener theories [2,3]. In recent times, quantum simulations of non-equilibrium dynamics of many-body spin systems have met with remarkable success. With improvement in atom trapping technology and owing to the long lifetime of Rydberg atoms, the number of atoms mimicking Ising type spin chains has increased from 51 to 200 within a short time [4,5], with the potential to observe different ordered phases with broken symmetry. Such tremendous experimental achievements make it possible to investigate the quantized nature of bubble nucleations in one and higher dimensions. Thus this work is of relevance for both current theoretical as well as experimental endeavors.

References

[1] https://arxiv.org/abs/2103.04762 - preprint.
[2] L. D. Landau, Phys. Zeit. der Sowj. 2, 56 (1932).
[3] C. Zener, Proc. R. Soc. Lond. A137, 696-702 (1932).
[4] A. Keesling et al.,Nature 568, 207 (2019).
[5] D. Bluvstein et al. , Science 371, 1355-1359 (2021)

Search for stable cocrystals of CL-20 using the evolutionary algorithm USPEX

Darya Snitavets

Moscow Institute of Physics and Technology

Poster #63

Hexanitrohexaazaisowurtzitane (CL-20) is a highly effective explosive that is hardly used because of its high sensitivity. A prospective way to decrease its sensitivity without loss in energetic characteristics can be cocrystallization of CL-20 with other molecules. In this work, the search for cocrystals of CL-20 with 1,4-dinitropiperazine, nitrogen dioxide, and dinitrogen tetroxide in molar ratios 1:1, 2:1, and 3:1 was performed. Minimization was carried out using the evolutionary algorithm USPEX. ReaxFF potential was used for the relaxation of the structures. Then energies of cocrystals were refined using the density functional theory with dispersion corrections (DFT-D3). Several stable structures were predicted.

Predicting new superconductor classes with Machine Learning methods

Timo Sommer

Karlsruhe Institute of Technology (KIT)

Poster #64

More than 100 years after the discovery of superconductivity in mercury, the search for new superconducting materials still largely remains a process of trial and error. The discovery of unconventional superconductors such as Cuprates and Ferrites stood in stark contrast to the theoretical beliefs at that time and came as a big surprise. In the last years, Machine Learning (ML) methods have emerged as a tool to potentially predict new materials for various applications. However, using ML approaches, new classes of superconductors have not been found so far, despite many attempts. In our work, we plan to predict the critical temperature of previously unknown classes of superconductors. In contrast to prior work we evaluate our model using Leave-One-Group-Out cross validation to get a reliable estimate of the extrapolation performance of our model to previously unknown classes of superconductors. To improve the extrapolation performance we additionally include information about the 3D structure of each crystal. We hope that our work will provide valuable insight into unknown patterns governing superconductivity, as well as provide a reliable estimate of the probability of a new material to be a superconductor with a specific critical temperature. Additionally we hope to come up with new insights into the relationship of different classes of superconductors. We anticipate that these findings will help researchers to narrow down the vast space of untested materials to find new superconductors.

Short-time Prediction of Heterogeneous Ice Nucleation via Molecular Dynamics and Machine Learning Approaches

Abhishek Soni

The University of British Columbia, Vancouver

Poster #65

Heterogeneous ice nucleation (HIN) is an important process in environmental, biological, and atmospheric science. A variety of mineral, organic, and biological materials function as ice-nucleating particles (INPs). Although an extensive amount of experiments have been performed, the microscopic features responsible for ice nucleation processes are still unclear. Molecular dynamics (MD) simulations of realistic model systems have begun to unravel some of the fundamental features of good INPs, however, the enormous amount of computational cost required to observe HIN in simulations is one of the immediate concerns. A major aim of current research is to utilize the machine learning (ML) tools combined with ice nucleation simulations of various atomistic substrates to predict the likelihood of HIN in a short amount of simulation time. Various features from MD simulations on diverse sets of substrates are extracted at a time interval where HIN has not even initiated. Our results suggest that combining surface properties along with the local water properties helps in classifying good/bad ice nucleators, with the water properties being dominant. The accuracy of our best classification model is 0.89 ± 0.05. The model selected sets of descriptors that can better predict the ice-nucleating ability of substrates. Some of the important ones are interfacial ice-like structures, hydrogen bonding to the surface, water density and water polarization near the surface, and the two-dimensional (2D) lattice match to ice developed in our lab. Finally, Principal Component Analysis (PCA) on the top 5 features selected by our model provides much better classification accuracy and the two classes are clearly separable. We believe that the approach followed here is an important step towards an understanding and prediction of ice nucleation (or lack thereof) by other surfaces.

Ground State Occupation of Single Atoms in Optical Tweezers

Stefan Spence

University of Durham

Poster #66

Optical tweezers offer precise control over both external and internal atomic degrees of freedom. The collisional blockade ensures trap occupancy of either one atom or none [1]. Using optical pumping we can control the atomic spin, and 2-photon Raman transitions can couple the spin with the harmonic levels of the trapping potential. Raman sideband cooling is now a standard technique for cooling atoms and has been used in optical tweezers to reach the ground state of the harmonic potential [2], which is a prerequisite to molecular association. The choice of Rabi frequency, trap frequency, pulse durations, and detunings for achieving high ground state fidelity is complicated when the atom's temperature means that it starts outside of the Lamb-Dicke regime and off-resonant excitation of the heating sideband is significant. Guided by simulations using QuTiP [3], some guiding physical principles, and M-LOOP [4], we present a choice of parameters that both achieves high ground state fidelity and is resistant against experimental imperfections.

[1] N. Schlosser et al., Nature, 411, 1024 (2001)
[2] A. Kaufman et al., Phys. Rev. X, 2, 041014 (2012)
[3] J. R. Johansson, P.D. Nation, and F. Nori, "QuTiP 2: A Python framework for the dynamics of open quantum systems", Comp. Phys. Comm. 184, 1234 (2013).
[4] Fast Machine-Learning Online Optimization of Ultra-Cold-Atom Experiments. Scientific Reports 6, 25890 (2016).

The photon: a discussion about its epistemic and ontic conceptual notion

Philipp Stammer

Institute of Photonic Sciences, Barcelona

Poster #67

The photon is a generic representation of a qubit and well studied in quantum theory. Its applicability in almost all quantum technologies requires its properties to be well defined and the understanding of its ontic and epistemic characteristics is indispensable. In this presentation we will talk about this notion of the photon. We discuss the question how the photon is defined in a meaningful way from an epistemological perspective. We show the necessity of taking into account the specific experimental configuration for relating the photons experimental evidence with ontic properties. By doing so, we have the delight to discuss the relation of an epistemic and ontic concept in quantum mechanics and to get a brief idea about the general aim of physical theory.

Electronic friction ML-based model for investigating nonadiabatic dynamics of hydrogen at Cu surface

Wojciech Stark

University of Warwick

Poster #68

The complexity of the dynamics of molecules at metal surfaces causes many discrepancies between classical methods and experiments. This has been credited mainly to the continuum of electronic states at metal surfaces. Classically, molecular dynamics methods are simplified by using Born-Oppenheimer approximation, which assumes that light electrons instantly follow movement of heavy nuclei. Nevertheless, dynamics of the molecules at metal surfaces can be much more complex due to electron-hole pair excitations. There are many methods to include such nonadiabatic effects, with one of the most efficient being molecular dynamics with electronic friction. Moreover, dynamics are also commonly affected by quantum effects, namely, by tunnelling and zero-point energy, which can be incorporated using path integral methods, like ring polymer molecular dynamics (RPMD). In this study we build unified ML-based electronic friction model for H2 on multiple Cu facets to study nonadiabatic effects at the metal surface with plan to combine it with RPMD.

Physics inspired nontrivial dynamics of learning

Nikita Stroev

Skolkovo Institute of Science and Technology

Poster #69

The deep learning (DL) paradigm invoked many intriguing questions concerning its underlying theory; however, DL effectiveness is of no question itself in many practical applications. Both active research and industrial activity are the causes of the great demand for specialized hardware, which can accelerate a tremendous amount of calculations. Thus, the search for alternative platforms suitable for the specific tasks even among unconventional physical systems begun. Exciton-polaritons, which are hybrid light-matter quasiparticles, are such condensed-matter systems that can be utilized to perform the dynamics on the so-called Lyapunov function with a specific problem of interest. However, the mathematical description of such dynamics is much more flexible and allow one to obtain several interesting regimes, some of which can give valuable insights into the learning process. We describe the associated mathematical model of such dynamics, cover most of the corresponding regimes and discuss the nonlinear deformations of the Lyapunov surface coming from the physical model.

Detecting ergodic bubbles at the crossover to many-body localization using neural networks

Tomasz Szołdra

Jagiellonian University in Kraków

Poster #70

Several theories of the ergodic to many-body localized transition suggest the existence of an avalanche mechanism, in which ergodic bubbles (local, thermal fluctuations of the system properties) thermalize their surroundings, leading to delocalization of the entire system, unless the disorder is sufficiently strong to suppress this process. We design a tool based on anomaly detection using neural networks that allows one to directly identify the ergodic bubbles using experimentally accessible two-site correlation functions. Studying time evolutions of the disordered Heisenberg spin chain, we observe a logarithmic in time growth of the ergodic bubbles in the MBL phase. Investigating the distributions of the bubble sizes, we find an exponential decay in the MBL regime and a power-law distribution with a thermal peak in the critical regime, confirming the presence of the avalanche mechanism. We also find quantitative differences in time evolution of chains with random and quasiperiodic disorder, as well as detect rare (Griffiths) events. These results open new pathways in the research of the mechanisms of thermalization in disordered many-body systems.

Investigation on the adsorption geometry of substituted aromatic compounds on the surface of Gold Nanoparticles: Quantum Chemical Topology and Vibrational Study

Rika Tandiana

Université Paris Saclay

Poster #71

Gold Nanoparticles (GNPs), owing to their unique optical properties and versatile preparation strategy, have been demonstrated to exhibit promising applications in diverse fields, which includes biosensors, catalysts, nanomedicines, bio-imaging, radiotherapy, and still many others.[1,2] Yet, the interfacial interaction of GNPs with their environment (ligand and solvent) remains elusive. The difference in experimental SERS spectra between closely related amino acids (tyrosine and phenylalanine) interacting on a metal surface (AgNP or AuNP), that arose due to difference in the orientation of the amino acid,[3,4] demonstrates the importance of understanding the interaction in greater details. However, the presence of multiple functional groups introduces competition, resulting in the complexity of such interactions. Therefore, it is our objective to systematically investigate the adsorption of small organic molecules on the surface of GNPs with varied functional groups to comparatively study their preference. In this study, we have systematically investigated the interaction between GNP and a series of substituted aromatic compounds that includes benzene, aniline, phenol, toluene, benzoic acid, acetophenone, methyl benzoate, and thiophenol.

Geometry optimization has indicated the preference of the benzene ring to lie flat on the surface for all of the systems, though for some molecules, the perpendicular orientation is possible thanks to the interaction with the functional groups, albeit with lower interaction energy. Then, the interaction energy and the charge transfer between the two fragments has been observed not to be directly correlated, regardless of the choice of population's scheme. Charge decomposition analysis also suggested back donation of electrons from GNP to organic molecules. A thorough quantum topological analysis has been performed to identify multiple non-covalent interactions and it revealed that the nature of the interaction includes dative interaction between the aromatic ring and GNP, as well as dispersive interactions. Lastly, the analysis of vibrational IR spectra has shown a significant change between the aromatic system oriented parallelly and perpendicularly at the surface of GNP, which would be an interesting distinction if observed experimentally as well.

References

1. Kuncic, Z.
Lacombe, S. Nanoparticle radio-enhancement: principles, progress and application to cancer treatment. Physics in Medicine & Biology 63, 02TR01 (2018).

2. Fen-Ying Kong et al. Unique Roles of Gold Nanoparticles in Drug Delivery, Targeting and Imaging Applications. Molecules 22, 1445 (2017).

3. Moskovits, M.
Suh, J. S. Surface selection rules for surface-enhanced Raman spectroscopy: calculations and application to the surface-enhanced Raman spectrum of phthalazine on silver. J. Phys. Chem. 88, 5526–5530 (1984).

4. Madzharova, F., Heiner, Z.
Kneipp, J. Surface Enhanced Hyper-Raman Scattering of the Amino Acids Tryptophan, Histidine, Phenylalanine, and Tyrosine. J. Phys. Chem. C 121, 1235–1242 (2017).

Quantifying information accumulation encoded in the dynamics of time series

Ying Tang

UCLA

Poster #72

Cellular responses to environmental changes are encoded in the complex temporal patterns of signaling proteins. However, quantifying the accumulation of information over time to direct cellular decision-making remains an unsolved challenge. This is, in part, due to the combinatorial explosion of possible configurations that need to be evaluated for information in the time series data. Here, we develop a quantitative framework, based on machine-learning models and inferred trajectory probabilities, to calculate the mutual information encoded in signaling dynamics while accounting for cell-cell variability. We use it to understand NFB transcriptional dynamics in response to different immune threats, and reveal that some threats are distinguished faster than others. The framework is generally applicable to single-cell time series measurements, and enables understanding how temporal regulatory codes transmit information over time.

Reconstructing the phase diagram of an interacting model from data of a non-interacting model through machine learning

Simone Tibaldi

University of Bologna

Poster #73

Neural networks are known for their generalization power and their recent success in applications to many fields of physics, including quantum many body physics. In this paper we investigate how far this generalization can be pushed by training a convolutional neural network (CNN) on a non-interacting model and testing it on its interacting Hamiltonian. The model we consider in this paper is the Kitaev model, a one dimensional chain of superconducting spinless fermions which exhibits topological phase transitions. We start by applying two machine learning algorithms, PCA and K-means on synthetic data of both models. We do this to understand which type of feature a neural network can exploit from the non-interacting data in order to predict the interacting one. Then we train a convolutional neural network on the non-interacting Kitaev model and test it on the non-interacting and the interacting one. By doing this the CNN is able to reconstruct both the phase diagram of the non-interacting and the interacting Kitaev model even being trained only on non-interacting data. This tool can be leveraged to investigate the unknown topological phases of an interacting model of which only the non-interacting phase diagram is known.

Computation of molecular excited states on IBM quantum computers using a discriminative variational quantum eigensolver

Jules Tilly

University College London

Poster #74

Solving for molecular excited states remains one of the key challenges of modern quantum chemistry. Traditional methods are constrained by existing computational capabilities, limiting the complexity of the molecules that can be studied or the accuracy of the results that can be obtained. Several quantum computing methods have been suggested to address this limitation. However, these typically have hardware requirements which may not be achieved in the near term. In this poster, I present a variational quantum machine learning based method to determine molecular excited states aiming at being as resilient as possible to the defects of early noisy intermediate scale quantum computers and demonstrate an implementation for H2 on IBM Quantum Computers. This method, inspired from the Generative Adversarial Machine Learning literature, uses a combination of two parametrized quantum circuits, working in tandem, combined with a variational quantum eigensolver to iteratively find the eigenstates of a molecular Hamiltonian.

Vortex Reconnections across the BCS-BEC Crossover

Marek Tylutki

Warsaw University of Technology (Politechnika Warszawska)

Poster #75

Reconnecting vortices in a superfluid allow for the energy transfer between different length scales and its subsequent dissipation. The present picture assumes that the dynamics of a reconnection is driven mostly by the phase of the order parameter, and this statement can be justified in the case of Bose-Einstein Condensates, where vortices have simple internal structure. However, less is known about this relation for the Fermi superfluids. Our findings show that the reconnection dynamics conforms with the predicted universal behaviour across the entire BCS-BEC crossover. The universal scaling survives also for spin-imbalanced systems, where unpaired fermions induce a complex structure of the colliding vortices.

Tuning ultracold collisions of He^*-Li with external magnetic field

Marcin Umiński

Nicolaus Copernicus University

Poster #76

One of the main goals of studying cold matter is to broaden our knowledge of mechanisms underlying chemical reactions. Recent advances in the field of cold matter experiments bring us closer to observing how chemical reactions may be precisely controlled. Feshbach resonances, which we observe in cold regime, are a quantum phenomenon playing a crucial role in the results of atom and molecule collisions. Alkali atoms and helium are good examples to observe due to their simple structures. Here we are examining a model system in which chemical reaction controlled by external field can be studied: the cold collisions of Li atoms with metastable helium (labelled as He^*) in magnetic field. He^*-Li molecules may come in one of two spin states: a stable, spin-polarized quartet state and unstable, low- spin doublet state, in which we observe the Penning ionization. The bound states are mixtures of these two states. To describe them we use two interaction potentials: a real, published before Morse/Long- Range potential describing quartet state and a predicted, theoretical complex potential of doublet state. To characterize the low-energy collisions we use the renormalized Numerov method and discrete variable representation. As we are interested in dependency on external magnetic field, we also consider Zeeman effect, which allows us to carefully shift Energy levels. Using this, we may tune our system to allow Feshbach resonances to happen. In proximity of resonances, we expect to observe increased rate of inelastic reactions, and thus ion production. Depending on the composition of these two states, the Feshbach resonances, which originate from them, might have different loss rates and shapes. Taking advantage of the mentioned properties we may, for the first time, observe chemical reactions induced by magnetic field.

Deep control of a quantum process from experimental data beyond interpolation: A use case of polarization in liquid crystals

Dominik Vašinka

Palacký University Olomouc

Poster #77

We explore the performance of deep neural networks in modeling quantum process transformations from partial measurements. Particularly, we focus on learning the transfer function of twisted nematic liquid crystals from random polarization measurements. We report unprecedentedly accurate preparation of arbitrary polarization state. Controlling polarization of light plays a crucial role in many applications, such as liquid crystal displays, polarization-sensitive imaging, and polarization encoding in optical communications and quantum information processing. Voltage-driven twisted nematic liquid crystals are widely used for fast polarization manipulation with a downside of limited accuracy, as their theoretical model lacks the necessary precision. Also, the model cannot be efficiently inverted to predict a control voltage required to perform a target operation. In our work, we aim to eliminate this obstacle using deep neural networks.

The developed network model predicts the control voltages required to prepare the desired polarization state by a liquid-crystal device with an average polarization fidelity of 99.96(5)%. This approach is more accurate than data interpolation and radial basis function model by two orders of magnitude. Furthermore, we study the model performance for a varying number of samples in the training dataset. We demonstrate scaling of the deep learning approach with the size of the experimental dataset outperforming both other methods considerably. We also report independent experimental verification of accurate arbitrary polarization preparation. Our results open the path to ultra-precise polarimetry using classical light as well as with single-photon signals. The accurate transformation of the polarization state of single photons is crucial to photonic quantum information processing. The developed approach can also be used for other degrees of freedom of light and controlling more complex quantum devices.

Physics-informed ML models for processing of spectroscopic data

Jakub Vrábel

CEITEC Brno University of Technology

Poster #78

Massive adoption of machine learning (ML) techniques in spectroscopy brought entirely new possibilities in analytical performance for applications, and also for basic research. However, several problems emerged, e.g. ML models are often utilized as "black-boxes", or considerably overtrained. Another issue is a blind transition of successful models (architecture, parameters) from distinct applications (e.g. image processing) to spectroscopic tasks, without taking into account the properties of data. We study the influence of (spectroscopic) data properties and incorporate them into ML models in form of weight initializations, specific parameter penalizations, and invariances. This leads to an increased analytical performance of models and better interpretability.

Estimating Posterior Distributions of Exoplanet Parameters with Conditional Invertible Neural Networks

Daniel Walter

Ruprecht Karl University of Heidelberg

Poster #79

Usually, exoplanet detection methods provide only sparse information about the internal planet structure. In some cases it is possible to determine the total mass M tot, the total radius R tot and the total ratios of magnesium to iron (M g/F e) tot and silicon to iron (Si/Fe) tot. Using data of a numerical forward model, we estimate posterior distributions of internal exoplanet parameters with a conditional invertible neural network (cINN).

Spin dynamics in ultracold collisions between Yb+ ion and Li atomsin the quantum regime.

Dariusz Wiater

University of Warsaw

Poster #80

Significant advances in precision measurements in the quantum regime have been achieved with trapped ions and atomic gases at the lowest possible temperatures. These successes have inspired ideas to merge the two systems [1]. Remarkably, in spite of its importance, experiments with ion-atom mixtures remained firmly confined to the classical collision regime, but recently buffer gas cooling of a single ion in a Paul trap to the quantum regime of ion-atom collisions has been realized[2]. The collision energy as small as 1.15(0.23) times the s-wave energy (or 9.9(2.0) K) has been achieved for a trapped ytterbium ion in an ultracold lithium gas. We have observed a deviation from classical Langevin theory by studying the spin-exchange dynamics, indicating quantum effects in the collisions.
Here, we present a theoretical description of the quantum ion-atom scattering used to guide and interpret the recent experiment [2]. By developing a theoretical model of measured energy-dependent spin-exchange rate constants, wenhave obtained singlet and triplet ion-atom scattering lengths. Next, we identify experimentally accessible Feshbach resonances in the mentioned systems and predict their properties. Control of both elastic scattering and related cooling rates, as well as inelastic spin-changing collisions, with the magnetic field is proposed and investigated to guide ongoing experimental efforts. Ion-atom Feshbach resonances in analogy to well-established techniques for neutral systems will be an important tool to manipulated ultracold ion-atom mixtures.

[1] Tomza et al, Rev. Mod. Phys. 91, 035001 (2019).
[2] Feldker et al, Nature Physics volume 16, pages 413–416(2020)

Revisiting the problem of the single hole in an antiferromagnet

Piotr Wrzosek

University of Warsaw, Faculty of Physics

Poster #81

Propagation of the single hole introduced into the antiferromagnetic ground state is one of the most studied problems in "cuprate physics", for it can be solved in a relatively controlled manner. Recently a renewed interest into this topic has been triggered by the possibility of simulating hole-doped antiferromagnets in the cold atom experiments [1]. In this contribution I would like to discuss some of our most recent studies on the propagation of the single hole in the antiferromagnet using the magnon language with a special attention paid to the interaction between the magnons [2-3]. To this end, I will introduce an intuitive picture which explains why the electron's spin and charge degrees of freedom can separate in a one-dimensional lattice, though a similar situation cannot occur in two dimensions [2]. Moreover, I will show that the string potential, which is believed to be felt by the hole moving in a two-dimensional Ising antiferromagnet, is significantly destroyed by the magnon-magnon interactions [3].

[1] C. S. Chiu et al., Science 365, 251 (2019); J. Koepsell et al., Nature 572, 358 (2019).
[2] K. Bieniasz et al., SciPost Phys. 7, 066 (2019).
[3] P. Wrzosek et al., Phys. Rev. B 103, 035113 (2021).

Non-adiabatic quantum reaction dynamics on coupled diabatic potential energy surfaces

Bin Zhao

Theoretical Chemistry, Faculty of Chemistry, University Bielefeld, Germany

Poster #82

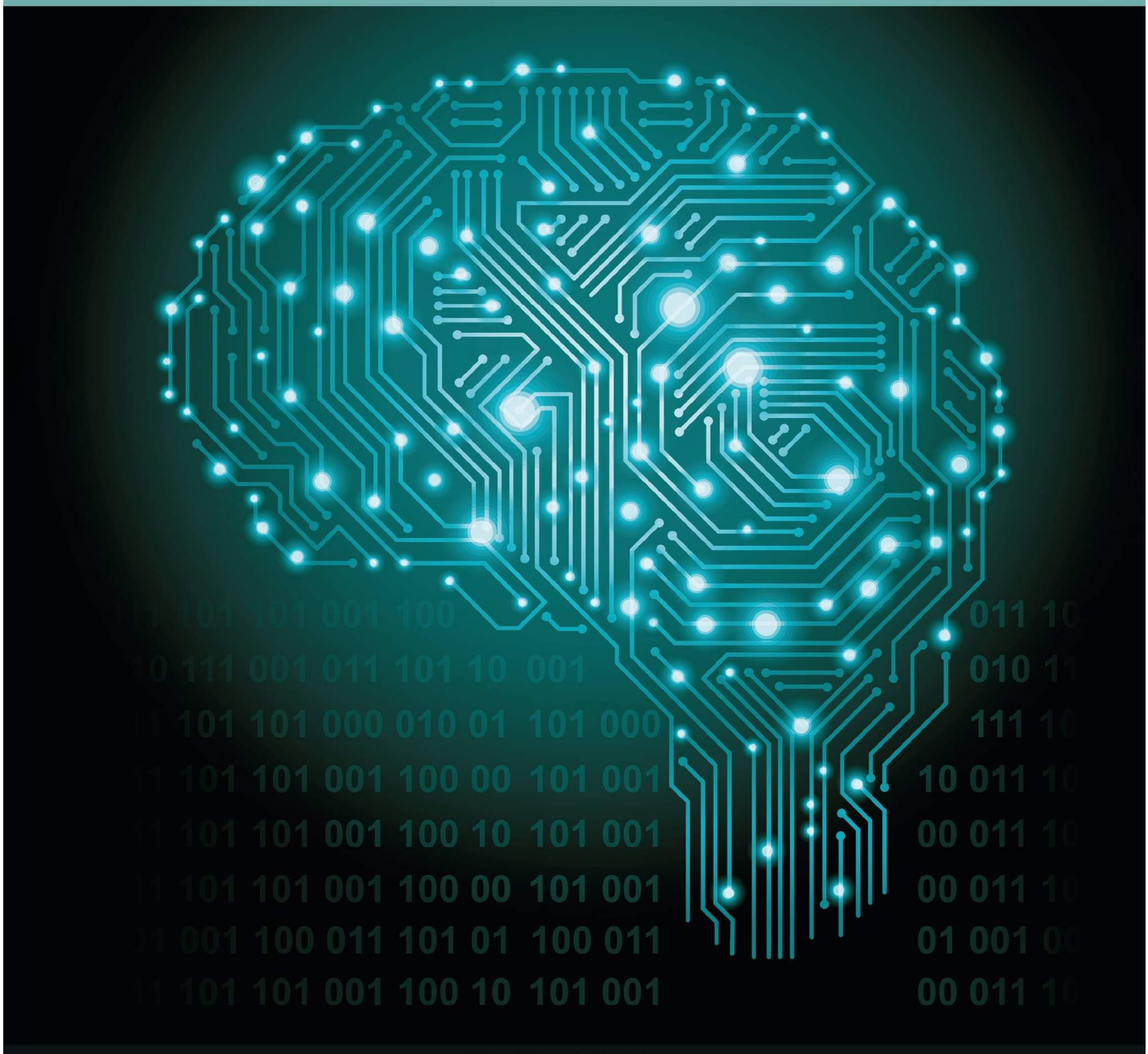
The Born-Oppenheimer (BO) approximation is often adopted to study chemical reactions in a single electronic state, thanks to the separable nuclear and electronic motion. However, the BO approximation breaks down for non-adiabatic dynamics that are impacted by several electronic states near an electronic degeneracy, such as a conical intersections (CI), where the electronic and nuclear coordinates are strongly coupled. While ultrafast nonadiabatic transitions near a CI have been extensively studied in photochemistry, fewer studies on non-BO effects exist for bimolecular reactions.

Here the non-adiabatic effects will be studied in two prototypical polyatomic reaction systems: (a) the nonadiabatic quenching of electronically excited OH(A) molecules by H2 molecules. This study reveals that the fate of OH(A)+H2 collision is largely determined by stereodynamics, namely the relative orientation between the two collisional partners. The quenching is made possible with the H2-OH approach as H2-HO collisions are ineffective in accessing the CI seam. (b) the effects of vibronic and spin-orbit couplings on the F(2P)+CHD3→HF+CD3 reaction. Non-adiabatic transitions are found to increase the reactivity compared to calculations within BO approximation and are more prominent than in triatomic reactions previously studied. Furthermore, the lifetimes of reactive resonances are reduced by non-adiabatic transitions.

MACHINE LEARNING

Science and Technology

iopscience.org/mlst



IOP Publishing