TT 2: Focus Session: Artificial Intelligence in Condensed Matter Physics I (joint session TT/DY)

While artificial intelligence leaves an ever growing footprint in our everyday lives, it has as well inspired various new approaches in the physical sciences; for instance, one of the outstanding success stories is the prediction of protein folding with unprecedented accuracy. But what role can AI play in condensed matter physics? This symposium aims to provide an overview and discussion of recent applications of modern machine learning and its prospects for the advancement of research in this field. The increasingly data-intensive experiments with high-dimensional observations call for the development of new tools for analysis matching known strengths of machine learning algorithms. Reinforcement learning agents can be employed to precisely manipulate many-body systems, which, among other use cases, is a pivotal ingredient for quantum technologies. On the computational side, ideas from deep learning and generative modeling inspire new building blocks to boost numerical simulations. One may even ask the question whether a machine can autonomously discover physical concepts such as effective degrees of freedom or equations of motion, and reveal them in an interpretable manner to human researchers.
Please note the second part of this session which will take place this afternoon, TT 14 (15:00 − 16:00) in the lecture Hall H3025.

Prof. Dr. Simon Trebst, Universität Köln
Prof. Dr. Florian Marquardt, Max-Planck-Institut Erlangen
Dr. Markus Schmitt, FZ Jülich

Time: Monday 9:30–13:15 Location: H 0104

Invited Talk TT 2.1 Mon 9:30 H 0104
Exploring artificial intelligence for engineered quantum matter — •Eliska Greplova — Kavli Institute of Nanoscience, Delft University of Technology, Netherlands

In research labs worldwide, quantum physics is making unprecedented strides. The realization of robust quantum systems holds tremendous promise for applications in secure communication and computing. Yet, as physicists, our most exciting pursuit lies in experimentally testing quantum phenomena predicted over the past century within highly controlled environments. In this talk, I will explore artificial intelligence approaches in the field of engineered quantum matter. Throughout the seminar, we will uncover how these approaches can be effectively deployed in contemporary quantum experiments. As one example, I will show how we can utilize generative models for parameter prediction of engineered topological systems known as Kitaev chains. Using this result and similar examples, I will discuss how we can use ML techniques to pave the way for advancing our control and understanding of real quantum experiments.

Invited Talk TT 2.2 Mon 10:00 H 0104
Communicability as a criterion for interpretable representations — •Renato Renner — ETH Zürich, Zürich, Switzerland

We propose an autoencoder architecture that can generate representations of data from physical experiments which are operationally meaningful and thus interpretable. The architecture is based on the paradigm of “communicability”. Roughly, the idea is that the encoder orders the data into several parts that may be communicated separately to agents, whose task is to answer different questions about the data. The encoding is then optimised so that this communication is minimised, i.e., each agent receives precisely the information that is relevant to its task. Using some toy examples, including ones from quantum state tomography, we show that this approach leads to a separation of parameters, which can be regarded as a step towards interpretability.

Invited Talk TT 2.3 Mon 10:30 H 0104
Disentangling Multiqubit States using Deep Reinforcement Learning — •Marin Bukov — Max Planck Institute for the Physics of Complex Systems

Quantum entanglement plays a central role in modern quantum technologies. It is widely perceived as a proxy for the quantum nature of physical processes and phenomena involving more than one particle. In this talk, we will revisit the problem of disentangling 4-, 5-, and 6-qubit quantum states with the help of machine learning techniques. We use policy gradient algorithms to train a deep reinforcement learning agent which, given access to the pure state of a multiqubit system, has to find the shortest sequence of disentangling two-qubit gates that brings it to a product state. We leverage the agent's interpolation and extrapolation capabilities to learn (approximately) optimal strategies to disentangle Haar-random states that lack any obvious spatial entanglement structure in the computational basis. Analyzing the protocols found by the agent, we show that any 4-qubit state can be prepared using at most 11 CNOT gates. Last, we also demonstrate the robustness of our agent to various sources of stochasticity common for present-day NISQ devices.

15 min. break

Invited Talk TT 2.4 Mon 11:15 H 0104
Neural Quantum States For The Many-Electron Problem — •Giuseppe Carleo — EPFL, Lausanne, Switzerland

This presentation explores recent strides in using neural quantum states [1] to represent many-body fermionic quantum wave functions for the many-electron problem [2]. I will delve into a message-passing-neural-network-based Ansatz designed for simulating strongly interacting electrons in continuous space [3]. This approach achieves unprecedented accuracy in the electron gas problem, pushing the boundaries of system sizes previously inaccessible to neural network states. I will also discuss a Pfaffian-based neural-network quantum state for ultra-cold Fermi gases, outperforming traditional methods and enabling exploration of the BCS-BEC crossover region [4]. Finally, I will provide insight into ongoing work on the entanglement properties of Helium 4 and Helium 3, and discuss open problems in the field [5].
[1] Carleo and Troyer, Science 355, 602 (2017)
[2] Hermann et al., Nature Reviews Chemistry 7, 692 (2023)
[3] Pescia et al., arxiv:2305.07240 (2023)
[4] Kim et al., arxiv:2305.08831 (2023)
[5] Linteau et al., in preparation (2024).

Invited Talk TT 2.5 Mon 11:45 H 0104
Neural quantum states for strongly correlated systems: learning from data and Hamiltonians — •Annabelle Bohrdt[1], Hannah Lange[2], Schuyler Moss[3], Fabian Döschl[2], Felix Palm[2], Giulia Semeghini[4], Mikhail Lukin[4], Sepehr Ebadi[4], Tout Wang[4], Fabian Grusdt[2], Juan Carrasquilla[5], and Roger Melko[3] — [1]Universität Regensburg — [2]LMU München — [3]UWaterloo — [4]Harvard University — [5]Vector Institute

Neural quantum states have emerged as a new tool to efficiently represent quantum many-body states with two main use cases: 1.) efficiently reconstruct a quantum state by training on measured data. For states with a non-trivial sign structure, measurements in many different basis configurations are necessary. I will present an active learning scheme which adaptively chooses the next measurement basis in order to maximize the information gain. 2.) The second main application of neural quantum states is to apply variational Monte Carlo to find e.g. the ground state of a system. I will present some of our recent results on ground states of strongly correlated systems, such as t-J type systems and fractional quantum Hall states. Finally, we combine both approaches: by first training on experimental data from a Rydberg atom tweezer array, we initialize the neural quantum state closer to the ground state. By then switching to variational Monte Carlo to minimize the energy in the second stage of training, we find a speedup in convergence. This showcases how limited datasets from experiments can be combined with numerical methods in a hybrid approach to yield more accurate results than either could provide on their own.

Invited Talk TT 2.6 Mon 12:15 H 0104

Towards an Artificial Muse for new Ideas in Quantum Physics — •Mario Krenn — Max Planck Institute for the Science of Light, Erlangen, Germany

Artificial intelligence (AI) is a potentially disruptive tool for physics and science in general. One crucial question is how this technology can contribute at a conceptual level to help acquire new scientific understanding or inspire new surprising ideas. I will talk about how AI can be used as an artificial muse in quantum physics, which suggests surprising and unconventional ideas and techniques that the human scientist can interpret, understand and generalize to its fullest potential.

[1] Krenn et al., Phys. Rev. X 11 (2021) 031044.
[2] Krenn et al., Nat. Rev. Phys. 4 (2022) 761.
[3] Krenn et al., Nat. Mach. Intell. 5 (2023) 1326

TT 2.7 Mon 12:45 H 0104

Adversarial Hamiltonian learning of quantum dots in a minimal Kitaev chain — •Rouven Koch[1], David van Driel[2,3], Alberto Bordin[2,3], Jose L. Lado[1], and Eliska Greplova[3] — [1]Department of Applied Physics, Aalto University, Espoo, Finland — [2]QuTech, Delft University of Technology, Delft, The Netherlands — [3]Kavli Institute of Nanoscience, Delft University of Technology, Delft, The Netherlands

Knowledge of the underlying Hamiltonian in quantum devices is key for tuning and controlling experimental quantum systems. Here we demonstrate an adversarial machine learning framework capable of Hamiltonian learning of a quantum dot chain from noisy experimental measurements. We train a convolutional conditional generative adversarial network with simulated data of the differential conductances based on a Kitaev chain model. The trained model is able to predict the parameters determining the sweet spot conditions of the two-quantum-dot system at which the predicted mid-gap bound state emerges. This gives us a fast and numerically efficient way to explore the phase diagram describing the transition between elastic co-tunning and Andreev reflection regimes and thus is suitable to assist the sweet-spot tuning of the Kitaev chains. The application of our methodology to experimental measurements in an InSb nanowire shows promising results in extracting Hamiltonians from measurements, potentially supporting the hard task of tuning quantum-dot systems into distinct Hamiltonian regimes.

TT 2.8 Mon 13:00 H 0104

Machine determination of a phase diagram with and without deep learning — •Burak Çivitcioğlu[1], Rudolf A. Römer[2], and Andreas J. Honecker[1] — [1]Laboratoire de Physique Théorique et Modélisation, CNRS UMR 8089, CY Cergy Paris Université, France — [2]University of Warwick, Coventry, UK

We study the performance of unsupervised learning in detecting phase transitions in the J_1-J_2 Ising model on the square lattice. We use variational auto encoders (VAE) and the reconstruction error, defined as the mean-squared error between two configurations, to explore the phase diagram of the system. Moreover, we propose as simple alternative method a direct spin comparison. The results of the spin comparison are contrasted with that of the VAEs. Our findings highlight that for certain systems, the simpler method can yield results comparable to a much more complex model, namely the VAE. This work contributes to the broader understanding of machine-learning applications in statistical physics and introduces an efficient approach to the detection of phase transitions using machine determination techniques.