DY 2: Focus Session: Physics Meets ML I – Machine Learning for Complex Quantum Systems (joint session TT/DY)

Modern machine learning methods open new perspectives on the high-dimensional data arising naturally in complex quantum systems. The applications range from the analysis of experimental observations over optimal control to the enhancement of numerical simulations in and out of equilibrium. This focus session brings together experts in the field to discuss recent progress and promising directions for future research.

Organizers: Markus Schmitt (University of Cologne), Martin Gärttner (University of Heidelberg)

Time: Monday 9:30–13:00 Location: HSZ 03

Invited Talk DY 2.1 Mon 9:30 HSZ 03

Enhanced variational Monte Carlo for Rydberg atom arrays — •Stefanie Czischek — Department of Physics, University of Ottawa, Ottawa, Canada, K1N 6N6

Rydberg atom arrays are promising candidates for high-quality quantum computation and quantum simulation. However, long state preparation times limit the amount of measurement data that can be generated at reasonable timescales. This restriction directly affects the estimation of operator expectation values, as well as the reconstruction and characterization of quantum states.

Over the last years, neural networks have been explored as a powerful and systematically tuneable ansatz to represent quantum wave functions. Via tomographical state reconstruction, such numerical models can significantly reduce the amount of necessary measurements to accurately reconstruct operator expectation values. At the same time, neural networks can find ground state wave functions of given Hamiltonians via variational energy minimization.

While both approaches experience individual limitations, a combination of the two leads to a significant enhancement in the variational ground state search by naturally finding an improved network initialization from a limited amount of measurement data. Additional specific modifications of the neural network model and its implementation can further optimize the performance of variational Monte Carlo simulations for Rydberg atom arrays and provide significant insights into their behaviour.

Invited Talk DY 2.2 Mon 10:00 HSZ 03

Data mining the output of quantum simulators – from critical behavior to algorithmic complexity — •Marcello Dalmonte — Abdus Salam International Centre for Theoretical Physics, Trieste (I)

Recent experiments with quantum simulators and noisy intermediate-scale quantum devices have demonstrated unparalleled capabilities of probing many-body wave functions, via directly probing them at the single quantum level via projective measurements. However, very little is known about to interpret and analyse such huge datasets. In this talk, I will show how it is possible to provide such characterisation of many-body quantum hardware via a direct and assumption-free data mining. The core idea of this programme is the fact that the output of quantum simualtors and computers can be construed as a very high-dimensional manifold. Such manifold can be characterised via basic topological concepts, in particular, by their intrinsic dimension. Exploiting state of the art tools in non-parametric learning, I will discuss theoretical results for both classical and quantum many-body spin systems that illustrate how data structures undergo structural transitions whenever the underlying physical system does, and display universal (critical) behavior in both classical and quantum mechanical cases. I will conclude with remarks on the applicability of our theoretical framework to synthetic quantum systems (quantum simulators and quantum computers), and emphasize its potential to provide a direct, scalable measure of Kolmogorov complexity of output states.

Invited Talk DY 2.3 Mon 10:30 HSZ 03

Reinforcement learning for quantum technologies — •Florian Marquardt — Max Planck Institute for the Science of Light and Friedrich-Alexander Universität Erlangen-Nürnberg, Erlangen, Germany

Complex quantum devices require sophisticated control. Discovering such control strategies from scratch with the help of machine learning will enable us to keep pace with the ever-increasing demands encountered when scaling up quantum computers. In this talk, I will describe how the field of reinforcement learning can deliver on this promise. I will present examples ranging from the optimization of quantum circuits to the model-based discovery of better quantum feedback strategies. Moreover, in a recent collaboration with our experimental colleagues, we could show how to train a novel latency-optimized neural network by reinforcement learning in an experiment, acting on a superconducting qubit in cycles of less than one microsecond.

Invited Talk DY 2.4 Mon 11:00 HSZ 03

Machine learning of phase transition — •Christof Weitenberg — Universität Hamburg, Institut für Laserphysik, Hamburg, Germany

Machine learning is emerging as vital tool in many sciences. In quantum physics, notable examples are neural networks for the efficient representation of quantum many-body states and reinforcement learning of preparation and read-out routines. In this talk, I will present our results on machine learning of quantum phase transitions using classification techniques. This approach works very well even on noisy experimental data both with supervised and unsupervised machine learning, as we demonstrate for quantum simulators based on ultracold atoms. Next to the practical advantages, such techniques might in the future reveal phase transitions, for which conventional order parameters are not known.

15 min. break

DY 2.5 Mon 11:45 HSZ 03

Machine learning optimization of Majorana hybrid nanowires — •Matthias Thamm and Bernd Rosenow — Institut für Theoretische Physik, Universität Leipzig

As the complexity of quantum systems such as quantum bit arrays increases, efforts to automate expensive tuning are increasingly worthwhile. We investigate machine learning based tuning of gate arrays using the CMA-ES algorithm for the case study of Majorana wires with strong disorder. We find that the algorithm is able to efficiently improve the topological signatures, learn intrinsic disorder profiles, and completely eliminate disorder effects. For example, with only 20 gates, it is possible to fully recover Majorana zero modes destroyed by disorder by optimizing gate voltages.

DY 2.6 Mon 12:00 HSZ 03

Model-independent learning of quantum phases of matter with quantum convolutional neural networks — •Yu-Jie Liu[1], Adam Smith[2], Michael Knap[1], and Frank Pollmann[1] — [1]Technical University of Munich, 85748 Garching, Germany — [2]University of Nottingham, Nottingham, NG7 2RD, UK

Quantum convolutional neural networks (QCNNs) have been introduced as classifiers for gapped quantum phases of matter. Here, we propose a model-independent protocol for training QCNNs to discover order parameters that are unchanged under phase-preserving perturbations. We initiate the training sequence with the fixed-point wavefunctions of the quantum phase and then add translation-invariant noise that respects the symmetries of the system to mask the fixed-point structure on short length scales. Without the translational invariance or other additional symmetries, we prove that a phase-classifying QCNN cannot exist. We illustrate this approach by training the QCNN on phases protected by time-reversal symmetry in one dimension, and test it on several time-reversal symmetric models exhibiting trivial, symmetry-breaking, and symmetry-protected topological order. The QCNN discovers a set of order parameters that identifies all three phases and accurately predicts the location of the phase boundary. The

proposed protocol paves the way towards hardware-efficient training of quantum phase classifiers on a programmable quantum processor.

DY 2.7 Mon 12:15 HSZ 03

Simulating spectral functions of two-dimensional systems with neural quantum states — •Tiago Mendes Santos[1], Markus Schmitt[2], and Markus Heyl[1] — [1]University of Augsburg, Augsburg, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Spectral functions are key tools to characterize and probe condensed matter systems. Simulating such quantities in interacting two-dimensional quantum matter is, however, still an outstanding challenge. This work presents a numerical approach to simulate spectral functions using Neural Quantum States. As the key aspect, our scheme leverage the flexibility of artificial-neural-network wave functions to access spectral properties by simulating the dynamics of localized excitations with the time-dependent variational Monte Carlo. For demonstration, we study the dynamical structure factor (DSF) of models describing two-dimensional quantum phase transitions, namely, the quantum Ising and a square-lattice Rydberg Atom Arrays model in a regime of parameters relevant to quantum simulators. When combined with deep network architectures whose number of variational parameters increase at a mild polynomial expense with the number of spins, we showcase that our approach reliably describes the DSF for unprecedented system sizes and time scales.

DY 2.8 Mon 12:30 HSZ 03

Efficient optimization of deep neural quantum states toward machine precision — •Ao Chen and Markus Heyl — Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

Neural quantum states (NQSs) have emerged as a novel promising numerical method to solve the quantum many-body problem. However, it has remained a central challenge to train modern large-scale deep network architectures, which would be key to utilize the full power of NQSs and to make them competitive or superior to conventional numerical approaches. Here, we propose a minimum-step stochastic reconfiguration (MinSR) method that reduces the optimization complexity by orders of magnitude while keeping similar accuracy as compared to conventional stochastic reconfiguration. In this talk, I will show MinSR allows for an accurate training on unprecedentedly deep NQS with up to 64 layers and more than 10^5 parameters in the spin-1/2 Heisenberg J_1-J_2 models on the square lattice. With limited numerical resources, partly obtained on single workstations, we find that this approach yields better variational energies as compared to existing NQS results and we further observe that the accuracy of our ground state calculations approaches different levels of machine precision on modern GPU and TPU hardware.

DY 2.9 Mon 12:45 HSZ 03

Time-dependent variational principle for quantum and classical dynamics — •Moritz Reh[1], Markus Schmitt[2], and Martin Gärttner[1,3,4] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany — [2]Institut für Theoretische Physik, Universität zu Köln, 50937 Köln, Germany — [3]Physikalisches Institut, Universität Heidelberg, Im Neuenheimer Feld 226, 69120 Heidelberg, Germany — [4]Institut für Theoretische Physik, Universität Heidelberg, Philosophenweg 16, 69120 Heidelberg, Germany

The solution of many-body quantum dynamics is a challenging feat due to the curse of dimensionality, hindering the exploration of dynamics beyond a mediocre number of qubits. Neural Networks can variationally approximate the state of interest and therefore present a promising tool as they allow to efficiently represent the quantum state at the expense of truncating the Hilbert space.

We present such a scheme that is aimed at solving dissipative quantum dynamics using a probabilistic framework, i.e. the so-called POVM-formalism and demonstrate it for spin chains of up to 40 spins. We then show that the generality of the approach allows us to translate this formalism directly to the case of partial differential equations in high dimensions, defeating the exponential growth of grid cells when adding dimensions.