

BACHELORARBEITEN SS 2022 – Themenliste

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- Understanding and Testing Quantum Decoherence
- Modelling collective behaviour with reinforcement learning

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- Sliding dynamics of a ring along closed polymer chains: A computational study on chains with topological constraints

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- Electronic properties of graphene moiré superlattices
- Machine learning of phase transitions

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- Dirac fermions on the lattice
- Machine learning, the inverse Ising problem and non-local Monte Carlo updates
- Finite-Size scaling at fixed renormalization-group invariant

BACHELORARBEITEN SS 2022 – Themenbeschreibungen**Univ.-Prof. Dr. Hans J. Briegel****Learning a state representation of quantum systems**

In this bachelor thesis, the student will create a neural network representation learning model to distill a representation of a quantum system from measurement data. To this end, they will form a basic understanding of concepts in quantum information theory such as density matrices and state tomography. They will create training data by simulating measurements on a random mixed quantum system and then train an autoencoder to learn a compressed (Bloch-)representation of the quantum system.

Example literature: Nielsen & Chuang, [Autoencoder implementations](#), [Representation learning in physics](#)

Understanding and Testing Quantum Decoherence

In this bachelor thesis, the student will explore the phenomenon of quantum decoherence by running and analyzing experiments on quantum hardware, e.g., available via the IBM Quantum Experience platform. To this end, they will form a basic understanding of concepts such as the density matrix formalism and common decoherence models in quantum computation. They will compare experiments run on quantum hardware to the predictions of a theoretical model of decoherence.

Example literature: Nielsen & Chuang, [IBM Quantum Composer](#)

Modelling collective behaviour with reinforcement learning

Reinforcement learning opens new possibilities to model individual animals as artificial learning agents, with their own perceptual apparatus and decision-making process. In addition, evolutionary pressures such as predation or the need for food can be encoded into the reward function, making the framework suitable for modelling complex scenarios where an ensemble of agents [1] interact with each other and with the environment [2,3,4,5]. In this project, the student will first study the reinforcement learning framework. A second goal will be to apply the framework to a concrete biological scenario, namely the collective defence of honeybee colonies [5].

Literature

- [1] L. Canese, et al., Appl. Sci. 11, 4948 (2021).
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- [3] M. Durve, et al., Phys. Rev. E 102, 012601 (2020).
- [4] A. López-Incera, et al., PLoS ONE 15(12), e0243628 (2020).
- [5] A. López-Incera, M. Nouvian, et al., BMC Biology 19, 106 (2021).

Univ.-Prof. Dr. Thomas Franosch**First-passage-time distribution of an active particle in a bistable potential**

Self-propelled particles are capable of converting energy into directed motion under certain non-equilibrium conditions. Examples of such agents are bacteria, protozoa, sperm cells, and synthetically designed microswimmers such as Janus particles, see Ref. [1].

A minimal model for such agents is the active Brownian particle model (ABP) where a particle moves along its axis with a constant propulsion speed, while the axis itself is subject to orientational diffusion [2]. Within this project we want to investigate by computer simulations the distribution of first passage times of such an agent in a paradigmatic double-well potential. If time permits, analytical approaches will also be discussed.

References

- [1] C. Bechinger et al, Active particles in complex and crowded environments, *Reviews of Modern Physics* 88, 045006 (2016).
- [2] C. Kurzthaler, S. Leitmann, and T. Franosch, Intermediate scattering function of an anisotropic active Brownian particle, *Scientific Reports* 6, 1 (2016).

Sliding dynamics of a ring along closed polymer chains: A computational study on chains with topological constraints

In recent years, rotaxanes (mechanically interlocked molecular architectures consisting of a ring which is threaded through a long polymer) and other mechanically interlocked molecular architectures have attracted much attention for their unique molecular dynamics and because of their relevance in biological systems and their potential as artificial new materials [1].

The most important feature of rotaxane is that the ring can move along the threaded chain generating fascinating sliding dynamics. While the sliding dynamics of rings along simple polymeric chains has been extensively studied [2,3], only very recently some attention was given to axial chains which are knotted [4].

In this project, the student will learn how to simulate polymeric systems and will investigate the diffusive motion of a small ring threading chains with non-trivial topological constraints, like knots and links to other chains [5], with the aim of understanding how the topology affects the properties of the rotaxane.

References

- [1] Leigh D.A., Marcos V., Wilson M.R., ACS Catal. 4 4490 (2014).
- [2] Yasuda Y., Toda M., Mayumi K., Yokoyama H., Morita H., and Ito K., Macromolecules 52 3787 (2019).
- [3] Li K., Wang Y.X., Guo F.C., He L.L., and Zhang L.X., Soft Matter 17, 2557 (2021).
- [4] Guo F.C., Li K., Wu J.X., Wang, Y.X., and Zhang, L.X., Polymer 235, 124226 (2021).
- [5] Caraglio M., Micheletti C., and Orlandini E., Scientific Report 7, 1156 (2017).

Univ.-Prof. Mag. Dr. Helmut Ritsch

Quantenoptik Simulationen mit der Julia Quantum Optics Toolbox

Julia is an open source programming language developed at MIT allowing efficient and easy to read framework for physics simulations. The additional package qojulia (<https://www.qojulia.org/>) developed in Innsbruck allows effective implementations of typical quantum optics Hamiltonians in Julia. This should be demonstrated in a generic example in this thesis.

Reference

- Krämer, S., Plankensteiner, D., Ostermann, L., & Ritsch, H. (2018). QuantumOptics.jl: A Julia framework for simulating open quantum systems. Computer Physics Communications, 227, 109-116.

A super-radiant laser as basis of new atomic clocks

A laser operating on a spectrally very narrow atomic transition can generate light of very precisely defined frequency and thus be the basis of a new type of atomic clocks. In this work a simple model of such a laser should be introduced and corresponding approximate numerical solutions calculated by help of the Julia Quantum Cumulants package <https://github.com/qojulia/QuantumCumulants.jl>

Reference

- Plankensteiner, D. et. al. "QuantumCumulants.jl: A Julia framework for generalized mean-field equations in open quantum systems." arXiv preprint arXiv:2105.01657 (2021).

Assoz. Prof. Mag. Dr. Wolfgang Dür

Messungsbasierte Verschränkungsreinigung

Quantenmechanische Verschränkung ist eine zentrale Ressource für viele Anwendungen im Bereich der Quanteninformationsverarbeitung. Die Herstellung von verschränkten Zuständen mit hoher Güte, insbesondere über große Entfernungen, ist aber schwierig. Verschränkungsreinigung stellt eine Möglichkeit dar, aus mehreren verrauschten Kopien von verschränkten Zuständen wenige Kopien mit einer höheren Güte zu erzeugen. Dazu wurden mehrere Verfahren entwickelt die in der Lage sind verschränkte Zustände zu reinigen. Üblicherweise ist dazu die Anwendung von kohärenten Operationen (Ein- und Zwei-qubit Gatter) notwendig. Ein alternativer Ansatz verfolgt die Verwendung von messungsbasierten Elementen für die Verschränkungsreinigung. Dabei werden bestimmte verschränkte Ressourcenzustände dazu verwendet, um die notwendigen Manipulationen alleinig durch Messungen durchzuführen. Dieses Verfahren ist dabei besonders robust gegenüber Rauschen und Imperfektionen. Ziel der Bachelorarbeit ist es, die zentralen Elemente dieses Zugangs zu erarbeiten, und eigenständig konkrete Beispiele auszuarbeiten und zu untersuchen.

Literatur

- C.H. Bennett, G. Brassard, S. Popescu, B. Schumacher, J.A. Smolin, and W.K. Wootters, Phys. Rev. Lett. 76, 722 (1996); (E-print: <https://arxiv.org/abs/quant-ph/9511027>).
- W. Dür and H.-J. Briegel, Rep. Prog. Phys. 70, 1381 (2007). (E-print: <https://arxiv.org/abs/0705.4165>).
- M. Zwerger, H. J. Briegel and W. Dür, Phys. Rev. Lett. 110, 260503 (2013). “Universal and optimal error thresholds for measurement-based entanglement purification”; (E-print: <https://arxiv.org/abs/1303.2852>).

Assoz. Prof. Dr. Wolfgang Lechner

QAOA

QAOA, short for “Quantum approximate optimization algorithm”, aims to find an approximate solution to combinatorial optimization problems. The performance of the algorithm is of great interest for near-term NISQ-devices (Noisy intermediate scale quantum), where proper error-correction methods are still out of reach. To implement optimization problems we use a technique based on the Ising model, which requires 4-body-interactions. This gives certain advantages and raises other challenges.

In this work you will understand and implement QAOA, while investigating different aspects of it.

Literature

- W. Lechner, P. Hauke, and P. Zoller, A quantum annealing architecture with all-to-all connectivity from local interactions, *Science Advances* 1 (2015).
- Lechner, Wolfgang. (2018). Quantum Approximate Optimization With Parallelizable Gates. *IEEE Transactions on Quantum Engineering*. 1. 10.1109/TQE.2020.3034798.
- E. Farhi, J. Goldstone, and S. Gutmann, A Quantum Approximate Optimization Algorithm, *arXiv:1411.4028* (2014).

Ass.-Prof. Dr. Gemma De las Cuevas**Universality & Undecidability everywhere**

Why is it so easy to generate complexity? Because essentially every non-trivial system is universal, that is, capable of exploring all complexity in its domain. In this sense there is ‘universality everywhere’ [1]. Here we will rigorously link the concept of universality in two domains: for spin models [2] and for automata (or, equivalently, formal languages) [3]. To this end, we will describe spin hamiltonians as automata, which will give rise to a new complexity measure of hamiltonians, with a different threshold between “easy” and “hard” than the computational complexity of the ground state energy problem [3]. In this project we will explore the consequences of this mapping.

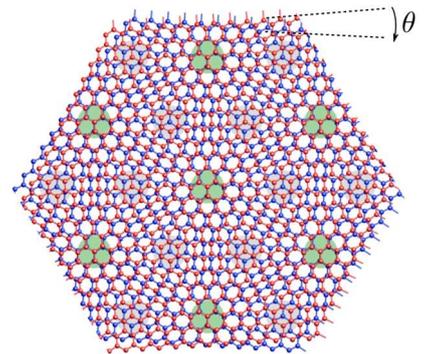
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- [1] G. De las Cuevas, FQXi Essay, <https://fqxi.org/community/forum/topic/3529>
- [2] G. De las Cuevas and T. S. Cubitt, *Science* 351, 1180 (2016).
- [3] Old version in D. Drexel and G. De las Cuevas, *arXiv: 2006.03529*.

Ass.-Prof. Dr. Mathias Scheurer

Electronic properties of graphene moiré superlattices

Graphene, a truly two-dimensional material consisting of a honeycomb arrangement of carbon atoms, has many interesting properties, probably best reflected in the 2010 Nobel prize of physics awarded for its experimental realization. In the last few years, it has been noticed that new and even more exciting systems can be designed by stacking several graphene layers with a finite relative twist angle. This leads to a spatial interference pattern – a so-called moiré superlattice (see figure) – and extraordinary electronic properties [1,2]. The study of graphene-based moiré systems has, thus, taken center stage in modern condensed matter research as a novel versatile playground for exotic many-body physics.



Using the pedagogical paper [3], we will learn how the electronic energy-momentum relation, also known as the bandstructure, of these systems can be computed. Depending on time, different approximations and/or setups (e.g., varying numbers of layers) will be explored.

References

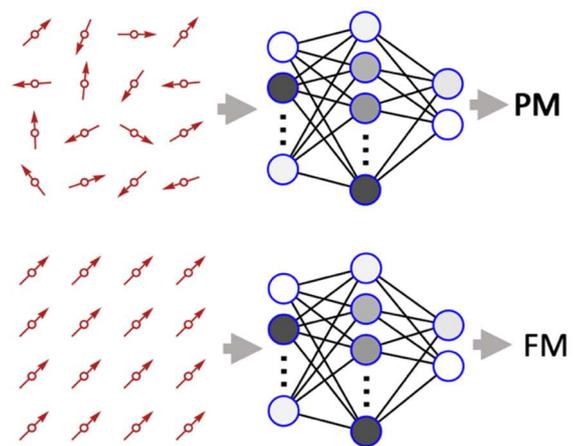
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- [2] MacDonald, Bilayer Graphene's Wicked, Twisted Road, Physics 12, 12 (2019).
- [3] Balents, General continuum model for twisted bilayer graphene and arbitrary smooth deformations, SciPost Phys. 7, 048 (2019).

Machine learning of phase transitions

The study of phase transitions is central to many fields of physics and chemistry. A classic example of a phase transition is the ferromagnet to paramagnet transition: in the paramagnetic phase (PM), the magnetic moments (for instance of electronic spins in a solid) are disordered such that the sum over all these moments, the so-called magnetization M , is zero. In the ferromagnetic (FM) phase, on the other hand, these moments spontaneously choose a preferred direction and M becomes non-zero. Since the value of M characterizes the transition, it is referred to as its order parameter.

Traditionally, the order parameter is constructed by hand based on physical intuition and then tested for a transition exhibited by a model of interest. However, motivated by the success of machine learning in a wide variety of applications, physicists have recently started to explore whether the study of phase transitions can be automated by machine learning techniques.

In this project, we will learn how to numerically generate data for simple models with phase transitions and to “train” certain machine-learning techniques to capture these transitions. Either basic neural-network approaches [1], based on “supervised learning”, or more sophisticated techniques [2], that work without prior human knowledge (“unsupervised learning”), can be explored.



References

[1] Carrasquilla & Melko, Machine learning phases of matter, Nature Physics 13, 431 (2017).

[2] Rodriguez-Nieva & Scheurer, Identifying topological order through unsupervised machine learning, Nature Physics 15, 790 (2019).

Dr. Thomas Lang, Senior Scientist

Dirac fermions on the lattice

This project's objective is to test and compare different implementations of lattice Dirac fermions, their topological properties and protections against perturbations and evaluate their practical applicability in future computer simulations.

Machine learning, the inverse Ising problem and non-local Monte Carlo updates

This project investigates the competitiveness of non-local updates learned via restricted Boltzmann machines, or designed via an effective model obtained from correlations for non-trivial interactions in classical and quantum models.

Finite-Size scaling at fixed renormalization-group invariant

This project scrutinises a recent suggestion to drastically improve the numerical finite size scaling analysis at classical and quantum critical points, which promises to pin down the critical properties of controversial phase transitions.