

BACHELORARBEITEN SS 2021 – THEMENLISTE

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- The Feynman-Kac formula
- Target-search problem: a comparison between intermittent searchers and active Brownian particles

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- Quantenfehlerkorrektur
- Quantum Computation

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- Der Laser als Modell einer Wärmekraftmaschine in der Quantenmechanik

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- The positivity problem in quantum many-body systems
- Universality everywhere: from spin models to automata

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- Machine learning of phase transitions
- Non-Hermitian many-body systems

Univ.-Prof. Dr. Thomas Franosch

The Feynman-Kac formula (für 2021 bereits vergeben – already assigned)

The Feynman-Kac formula, authored by Richard Feynman and Mark Kac, is an important mathematical result which provides a representation of the solutions of some classes of partial differential equations (PDE) using the probabilistic properties of stochastic processes.

The application of Feynman-Kac formula plays an important role in many applications in different fields including statistical mechanics, biology and finance [1]. In this project the student will learn to master the Feynman-Kac for solving partial differential equation in electrostatics. In particular, he/she will use the method to solve the problem of concentric spherical capacitor and will compare the results with the known analytical solution. Then, building on this first step, he/she will move to more complex problems for which the analytical solution is not known or it is more difficult to obtain. A first possible example will be the problem of two spherical capacitors which are not concentric.

References:

[1] Del Moral Pierre, Feynman-Kac Formulae: Genealogical and Interacting Particle Systems with Applications, Springer Science & Business Media (2012).

Target-search problem: a comparison between intermittent searchers and active Brownian particles (für 2021 bereits vergeben – already assigned)

One of the most common every-day challenges that living beings have to face is that of finding the best strategy to reach a target. For bacteria and animals, this usually concerns looking for food or mate, while for humans it could simply mean searching for lost keys. More generally, the search problem is a universal question arising at different scales and in various fields [1]. Other relevant examples include phagocytes of the immune system pursuing health threats [2], sperm cells navigating against chemical gradients to find the egg [3], and artificial nanoparticles that may act as drug delivery agents [4].

Among the various search strategies that can be used, intermittent search strategies (i.e. strategies combining phases of diffusive motion allowing target detection and phases of ballistic motion that allow moving quickly to a different region but do not allow to detect the target) have been widely studied because they are observed in nature at various scales [1]. Another successful model for bacteria motion is the active Brownian particle (ABP) model [5,6]. However, much less is known about the performances and behavior of ABPs in target-search problems.

In this project, the student will learn how to simulate intermittent search particles and ABPs in two dimensions with the goal of studying their target-search behavior and make a comparison between the two models in this context.

References:

- [1] O. Bouchou, C. Loverdo, M. Moreau, and R. Voituriez, Rev. Mod. Phys. 83, 81 (2011).
- [2] P. N. Devreotes and S. H. Zigmond, Annu. Rev. Cell Biol. 4, 649 (1988).
- [3] M. Eisenbach and L. C. Giojalas, Nat. Rev. Mol. Cell Biol. 7, 276 (2006).
- [4] S. Naahidi, M. Jafari, F. Edalat, K. Raymond, A. Khademhosseini, and P. Chen, J. Control. Rel. 166, 182 (2013).
- [5] C. Bechinger, R. Di Leonardo, H. Löwen, C. Reichhardt, G. Volpe, G. Volpe, Rev. Mod. Phys. 88, 045006 (2016).
- [6] P. Romanczuk, M. Bär, W. Ebeling, B. Lindner, and L. Schimansky-Geier, Eur. Phys. J. Special Topics 202, 1 (2012).

Univ.-Prof. Mag. Dr. Barbara Kraus

Quantenfehlerkorrektur

Fehler treten in jeder quantenmechanischen Berechnung auf. Ohne die Möglichkeit diese Fehler zu korrigieren wäre eine quantenmechanische Berechnung nicht sehr nützlich. Ziel dieser Bachelorarbeit ist es Methoden zur Fehlerkorrektur zu erlernen.

Literatur:

- [1] M. Nielsen, I. Chuang, Quantum Computation and Quantum Information, Cambridge, UK: Cambridge University Press

Quantum Computation

Ziel ist es einige wichtige Quantenalgorithmien, wie z.B. Deutsch- Jozsa, Grover, Shor zu verstehen.

Literatur:

- [1] M. Nielsen, I. Chuang, Quantum Computation and Quantum Information, Cambridge, UK: Cambridge University Press

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.

A laser as a quantum model of a heat engine

A single mode laser can be seen as a heat engine converting high temperature thermal radiation to a single mode coherent field of vanishing entropy. At the hand of a single or a few three level atoms coupled to thermal reservoirs and a cavity mode, the underlying concepts should be explained and the efficiency and power of the operation studied.

[1] Boukobza, E., and H. Ritsch, *Physical Review A* 87.6 (2013): 063845.

Univ.-Prof. Dr. Oriol Romero-Isart

Theory and simulation of spin waves in a ferromagnet

Magnets are fascinating objects and key ingredients in current technologies. They support the propagation of spin waves, namely magnetization fields with intriguing and tunable properties. Understanding these complex waves is of strategic interest for applications in future information technologies and hybrid quantum systems. In particular, theoretically determining the spin wave eigenmodes supported by a magnetic structure is key for these applications. However, for many geometries of experimental interest this problem becomes analytically intractable and requires advanced numerics.

In this project, the student will calculate the spin wave eigenmodes of a thin magnetic disk, a configuration used in many experiments. They will first learn the analytical techniques [1] and compute the eigenmodes for a perpendicularly magnetized disk. The student will then numerically calculate the non-analytical eigenmodes of a tangentially magnetized disk using advanced micromagnetics software [2].

[1] D. Stancil, A. Prabhakar, "Spin waves: theory and applications", Springer US (2009)

[2] <https://mumax.github.io>

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. Zwirger, 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

Adiabatic Quantum Computing

Das Ziel eines adiabatischen Quantencomputers ist es, quantenmechanische Eigenschaften wie Superposition, Verschränkung und Tunneln zu verwenden, um Optimierungsprobleme zu lösen. Dies können klassische Optimierungsprobleme sein (wie das Traveling Salesman Problem) oder quantenmechanische Probleme (wie Elektron-Grundzustände in Molekülen). In dieser Bachelorarbeit verwenden wir einen adiabatischen Quantencomputer, der auf einem Ising-Modell mit 4-Körper-Wechselwirkungen basiert. Diese bestimmte Art der Wechselwirkung kann dazu verwendet werden neue Protokolle zu entwickeln, die z.B. für künstliche Intelligenz relevant sind. Konkret soll in der Bachelorarbeit ein adiabatisches Protokoll entwickelt und optimiert werden. Aus den theoretischen Ergebnissen sollen Vorschläge für experimentelle Implementierungen entstehen.

Voraussetzung: gute Kenntnisse der Quantenphysik

Ass.-Prof. Dr. Gemma De las Cuevas

The positivity problem in quantum many-body systems

The positivity problem in quantum many-body systems is the difficulty of representing a quantum mixed state efficiently. Namely, mixed states are described by positive semidefinite matrices, but efficient representations of mixed states do not make the positivity of the state explicit [1], and this leads to many problems. Recently it was found that this problem is related to several other problems in mathematics, in particular to decompositions of nonnegative matrices [1,2]. In this work we will analyse several of these connections to gain insight into the positivity problem.

[1] G. De las Cuevas and T. Netzer, Mixed states in one spatial dimension: decompositions and correspondence with nonnegative matrices, arXiv:1907.03664

[2] G. De las Cuevas, M. Hoogsteder Riera and T. Netzer, Tensor decompositions on simplicial complexes with invariance, arXiv:1909.01737

Universality everywhere: from spin models to automata

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’. Here we will rigorously link the concept of universality in two domains: for spin models [1] and for automata (or, equivalently, formal languages) [2]. 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 [2]. In this project we will explore the consequences of this mapping.

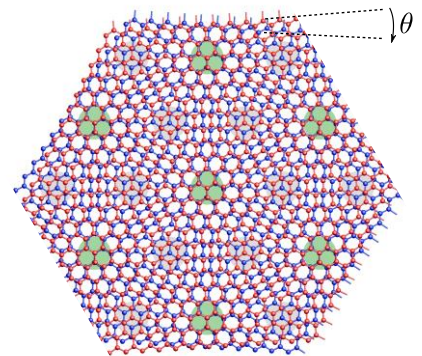
[1] G. De las Cuevas and T. S. Cubitt, Science 351, 1180 (2016).

[2] D. Drexel and G. De las Cuevas, upcoming.

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.



The goal of this project is to learn how the electronic energy-momentum relation, also known as the bandstructure, of these systems can be computed within the free-electron approximation. Different setups can be explored, e.g., varying numbers of graphene layers and twist angle configurations.

[1] Gast, Der Magische Winkel, Spectrum der Wissenschaft, 2019.

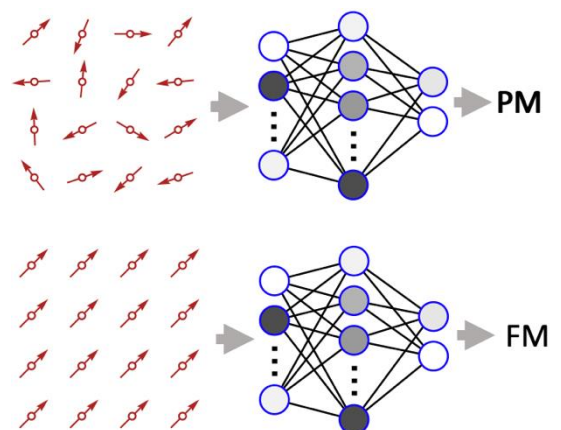
[2] MacDonald, Bilayer Graphene’s Wicked, Twisted Road, Physics 12, 12 (2019).

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.

[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).

Non-Hermitian many-body systems

Very early on in your quantum mechanics class, you learned that the Hamiltonian of a quantum system has to be Hermitian, which is related to the unitarity of or, more physically, probability conservation under time evolution. However, many effective descriptions of physical systems, such as open quantum systems, turn out to be governed by Schrödinger-like equations with non-Hermitian Hamiltonians. Non-Hermitian Hamiltonians exhibit many unique features, such as non-orthogonal eigenstates and exceptional points [1] with interesting physical consequences. While significant progress has been made in understanding non-Hermitian single-particle quantum mechanics, in particular, for so-called PT-symmetric systems [2], non-Hermitian many-body quantum physics has remained much less explored but is being established as a very rich emergent field (see figure).

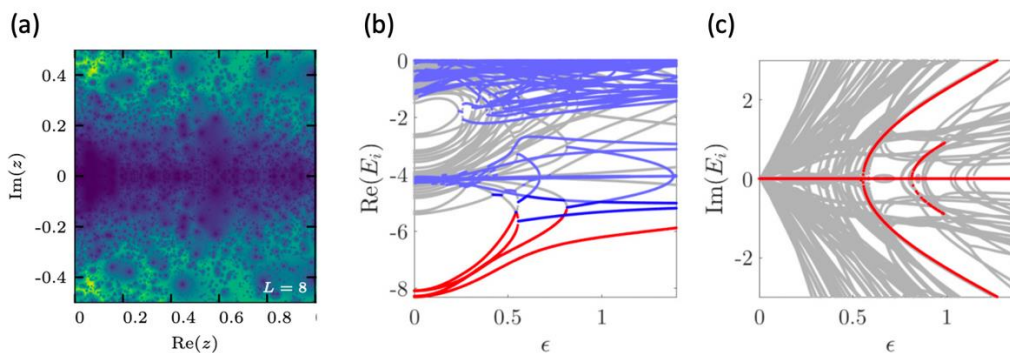


Figure: While (a) exceptional points proliferate exponentially in generic many-body systems [3], certain classes (b,c) of models have been shown to exhibit protected subspaces (red) [4].

The first goal of this project is to learn the basics of non-Hermitian quantum mechanics. We will then numerically study the behavior of a few interesting many-body systems upon introducing non-Hermitian terms.

[1] Heiss, The physics of exceptional points, *J. Phys. A: Math. Theor.* 45, 444016 (2012).

[2] Bender, Making sense of non-Hermitian Hamiltonians, *Rep. Prog. Phys.* 70, 947 (2007).

[3] Luitz & Piazza, Exceptional points and the topology of quantum many-body spectra, *Phys. Rev. Research* 1, 033051 (2019).

[4] Shackleton & Scheurer, Protection of parity-time symmetry in topological many-body systems: Non-Hermitian toric code and fracton models, *Phys. Rev. Research* 2, 033022 (2020).