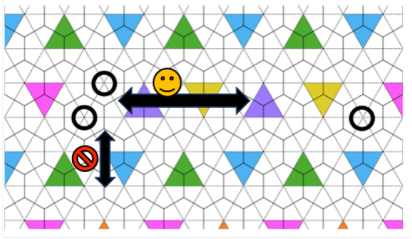
Masters Thesis Projects 2025

Theory of Quantum Matter, Prof. Titus Neupert

Investigate emergent fracton behavior in two dimension

Excitations with restricted mobility are features of fracton topological phases of matter, which have gained lots of theoretical interest in recent years due to their potential application as robust quantum memory in quantum computation. Although there is no stable fracton topological order in two dimension, whether there can be emergent fracton dynamics at low energy is an interesting question. A previous study has shown that sub-dimensional dynamics can emerge in a 2D quantum system with cluster charging interaction (see Figure), but the nature of such dynamics remains unknown. We aim to tackle this problem in this project. The planned research will start with the 1D limit of the 2D problem, investigating the quantum phase diagram of a single chain, using both analytical and numerical methods such as Bethe ansatz and density-matrix renormalization group (DMRG). After gaining knowledge about a single chain, multiple rungs will be considered, aiming toward the physics of a full 2D system. Experimental observables such as conductivity and tunneling density of states will be discussed, aiming towards providing falsifiable predictions that can guide future experiments.



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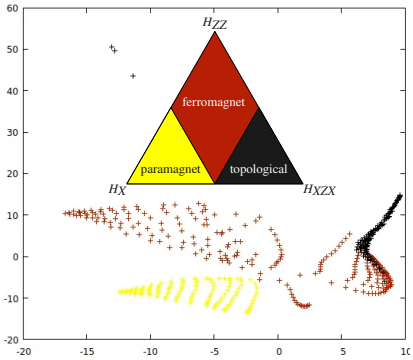
Keywords: Fracton, cluster charging interaction, Bethe ansatz, DMRG

Classification of topological phases with neural networks

Machine learning has had great success in classifying and recognising patterns in a variety of inputs. This includes classifying phases of matter based on data from experiments or simulations. However, there exist exotic phases known as topological phases, which are indistinguishable from trivial noninteracting states by straightforward local measurements, even though they carry intricate patterns of quantum correlations and entanglement.



In this project, you will explore whether machine-learning techniques can distinguish symmetry-protected topological (SPT) phases from conventionally ordered and disordered ones through the example of a spin-chain Hamiltonian. You will learn about principal component analysis (PCA) and variational autoencoders (VAEs), tools designed to extract similarities and differences from data, as well as the DMRG algorithm for efficiently computing ground states of interacting quantum Hamiltonians. You will study whether these tools can distinguish the phases through conventional measurements (e.g., correlation functions).

An exciting outlook for an ambitious student will be exploring direct quantum measurements (i.e., samples from the Born probability distribution) as input data. This connects readily to experiments done on quantum simulators and promises interesting mathematical challenges in implementing a VAE that works directly with the Born distribution.

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Keywords: Machine learning, topological phases, variational autoencoder, probability theory

Anderson-Higgs mechanism in quantum spin liquids

Quantum spin liquids are exotic phases of matter with long-range entanglement, which allows electrons in the material to separate their electric charge and spin into two independent particles. Some of these systems are also topologically ordered, in which these particles go beyond the usual split between bosons and fermions to realise anyonic statistics. While field theory predicts an abundance of such topologically ordered systems, they have been challenging to realise in microscopic models: most of these favor simpler spin liquids, or the length scale for topological order is too large for most numerical methods.

In this project, you will explore the origin of this discrepancy in the field theories that describe quantum spin liquids. In these, the particles carrying spin are coupled to a number of emergent gauge fields: realising topological order requires all of these to be suppressed through the Anderson-Higgs mechanism, similar to how superconductors do not allow magnetic flux to enter them. While this happens generically, it is plausible that some gauge fields are more weakly suppressed than others, able to survive over large length scales and to mask the eventual topological order. The bulk of the project will consist of developing analytical field-theory methods to describe this mechanism; you will also implement its results computationally to study a few models of experimental interest in more detail.

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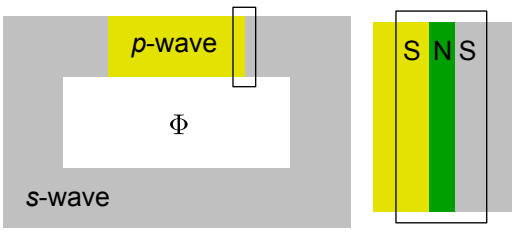
Keywords: Quantum spin liquids, topological order, Anderson-Higgs mechanism, superconductivity, gauge theory

Spin-triplet superconductivity and the Little-Parks effects

The Little-Parks effect describes how a flux Φ piercing a superconducting ring changes the superconducting transition temperature T_c periodically with period $\Phi_0 = h/2e$, where the maximum in T_c occurs at zero flux. If the ring is composed of superconductors of different pairing symmetry, the maximum can in principle move, but unless time-reversal symmetry is broken, zero flux will correspond to a maximum or a minimum. While the matrix elements for coupling spin-singlet superconductors of different pairing symmetry are rather straight-forward to evaluate, the situation is less clear when we couple a spin-singlet and spin-triplet superconductor (see Figure).



Left: Setup of the composite-ring Little-Parks setup. Right: SNS junction to study matrix elements in the spin-triplet spin-singlet setup.

In this project, we want to study the matrix elements and their effect on the Little-Parks effect for ring geometries that involve spin-singlet and spin-triplet superconductors. For this purpose, we will first focus on a superconductor–normal metal–superconductor (SNS) junction including a spin-triplet superconductor to understand the matrix elements (see Figure). This situation can be analyzed within the Andreev approximation, but can later be extended to microscopic calculations in the form of tight-binding calculations.

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Keywords: Unconventional Superconductivity, Josephson coupling, Little-Parks effect, Andreev approximation.

Spatially modulated superconductivity and disorder

Many superconducting materials exhibit a phase diagram where superconductivity emerges on top of a charge density wave (CDW) background, a state characterized by a redistribution of charge that breaks translational symmetry. This symmetry breaking naturally leads to a spatial modulation of the superconducting order, which can be described by a homogeneous order together with a pair density wave (PDW) component. With advancements in experimental techniques, such as the scanning tunneling microscope, these modulations in the superconducting order have been observed in several systems. One notable example is the recently discovered family of kagome material, AV_3Sb_5 (A = K, Rb, Cs), which displays both superconductivity and CDW order. In this project, we aim to theoretically explore the experimental signatures of such superconducting states, with a particular focus on how they respond to disorder in the material.

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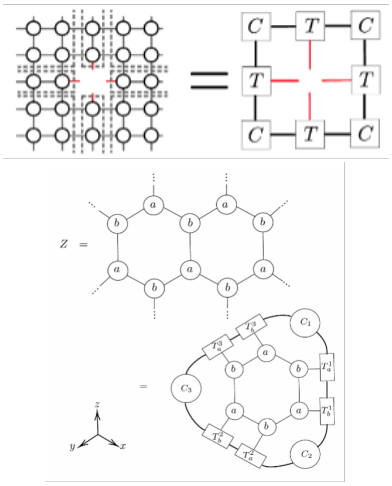
Keywords: Superconductivity, charge density wave, pair density wave, spatial modulation

Spatially-symmetric tensor networks for triangular lattice

A key step in evaluating expectation values within the infinite Projected Entangled-Pair States (iPEPS) framework is the Corner Transfer Matrix (CTM) algorithm, which enables the approximate contraction of formally infinite tensor networks. Traditionally, iPEPS simulations have utilized networks with square lattice geometry, required by CTM. While this approach can be adapted for models on the triangular lattice, it does not allow for the straightforward imposition of the triangular lattice's point group symmetries. Recently, a new variant of the CTM algorithm has been developed for the honeycomb lattice [4], which is the dual of the triangular lattice. This result opens a path to tensor network simulations which retain the point group symmetries of triangular lattice. The goal of this project is to implement such symmetric iPEPS and the corresponding CTM algorithm and benchmark its performance against current state-of-the-art results for the Heisenberg model on the triangular lattice.



CTM environments of infinite square (up) and honeycomb (down) lattices

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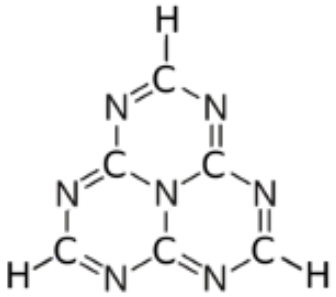
Keywords: Tensor networks, iPEPS, CTM algorithm, triangular lattice model

Optical properties of small molecules beyond single reference with tensor networks

The modeling of small molecular systems is a well-established field in precision quantum chemistry. Computer simulations of such systems typically employ methods ranging from Density Functional Theory (DFT), which describes the ground state using a single Slater determinant, to Coupled Cluster (CC) methods, which superpose a reference Slater determinant with perturbations involving single, double, or higher particle-hole excitations. However, multireference problems—where no single Slater determinant dominates the electronic ground state—pose

a particular challenge. For these systems, a tensor network approach based on Matrix Product States (MPS) offers an efficient alternative, as it can effectively capture complex electronic wavefunctions. In this framework, the kinetic energy and Coulomb interactions are encoded in an effective Hubbard model on a fully connected graph formed by all considered atomic orbitals. By selecting an appropriate orbital ordering, the ground state can be directly expressed and optimized as an MPS, with a computational cost scaling of $O(N^4)$.



A heptazine molecule $C_6H_3N_7$

This project aims to develop a workflow for simulating ground and excited states of small molecular systems and to estimate the computational resources required for such simulations, leveraging established MPS software. A motivating case study is a heptazine, an organic molecule of significant interest due to its unusual singlet-triplet inversion. In these systems, the energies of the lowest singlet and triplet excited states violate Hund's multiplicity rule—a rare phenomenon in stable organic molecules, with significant implications for their photophysics and photochemistry.

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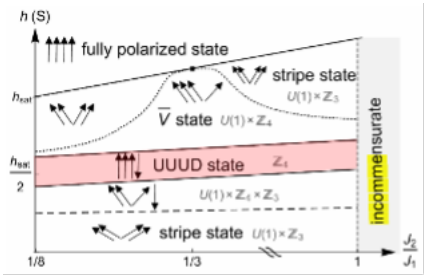
Keywords: Slater determinant, Tensor Network, Matrix Product States

Spirals and spin liquids in extended antiferromagnetic Heisenberg model on triangular lattice

Antiferromagnetic Heisenberg model on a triangular lattice is a reference problem in frustrated magnetism, subjected to intense scrutiny for past decades in search of exotic states of quantum matter: from resonating valence bond theory proposed in the 70's by Fazekas and Anderson to a contemporary Dirac spin liquid once next-nearest neighbour interaction comes into play. In this regard, great effort has been dedicated to the study of highly-frustrated regions where the nearest-neighbor J_1 and next-nearest neighbor J_2 spin exchanges are in the ratio $J_2/J_1 \approx 1/8$. However, the region where $J_2 > J_1$ remains largely unexplored, partly due to the challenges posed by the incommensure order suggested by semiclassical analysis. Recently developed spiral iPEPS provide a powerful framework for studying such systems, as they can effectively model magnetic orders without being constrained by the spatial wavelength of magnetic textures. The goal of this project is to investigate the stability of the incommensurate phase predicted by semiclassical theory and establish the phase diagram for large J_2/J_1 ratios.



Semiclassical phase diagram of antiferromagnetic Heisenberg model on triangular lattice in external magnetic field

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Keywords: Heisenberg model, frustrated magnetism, Dirac spin liquid, iPEPS