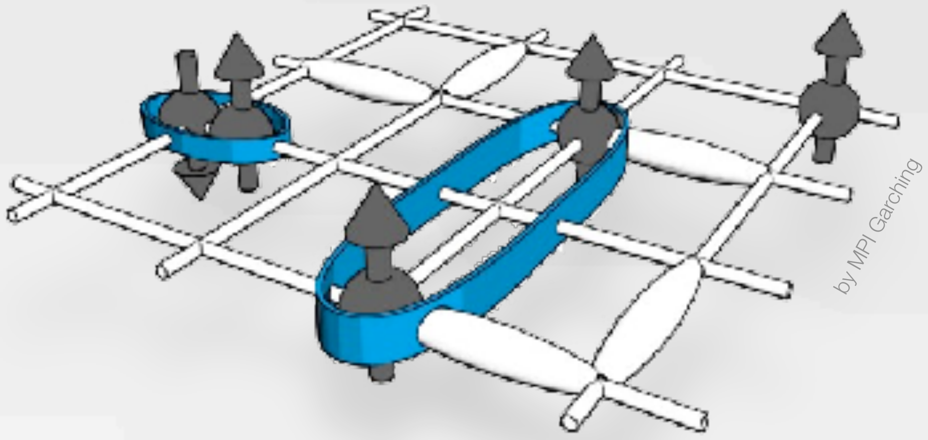
Theoretical condensed matter & Computational physics

Bachelor thesis projects

We numerically investigate strongly correlated quantum many body systems in crystalline materials, optical traps and models, where two or more interactions are competing against each other at the same energy scale.



by MPI Garching

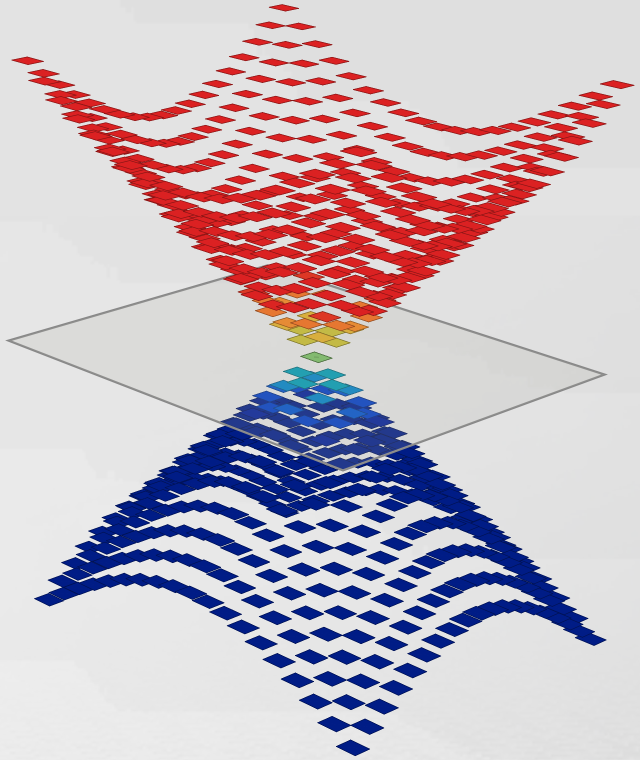
Research in this area attempts to model and simulate existing materials, as well as to predict the properties of designer materials and models.

Our challenge is to understand the fundamental, complex interplay of many degrees of freedom, which can lead to exotic states of matter.

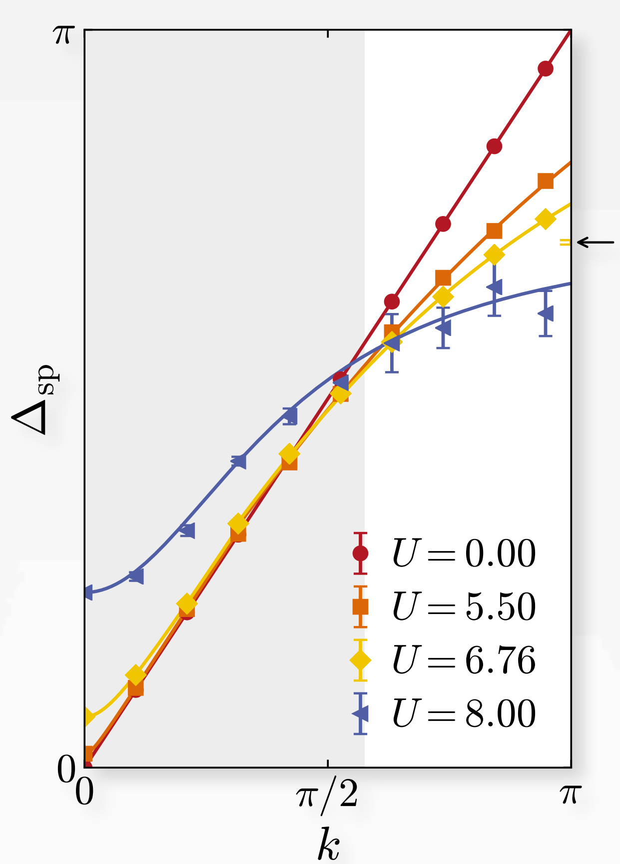
VSC4

Dirac fermions on the lattice

Relativistic Dirac fermions constitute the fundamental starting point and building block for a vast host of modern physics topics, from twisted multilayer graphene to topologically protected surface states.



Implementing an effective relativistic energy-momentum relation for Dirac fermions in computer simulations remains however a technical challenge, which haunts high energy physics, condensed matter physics, but also cold atom experiments.

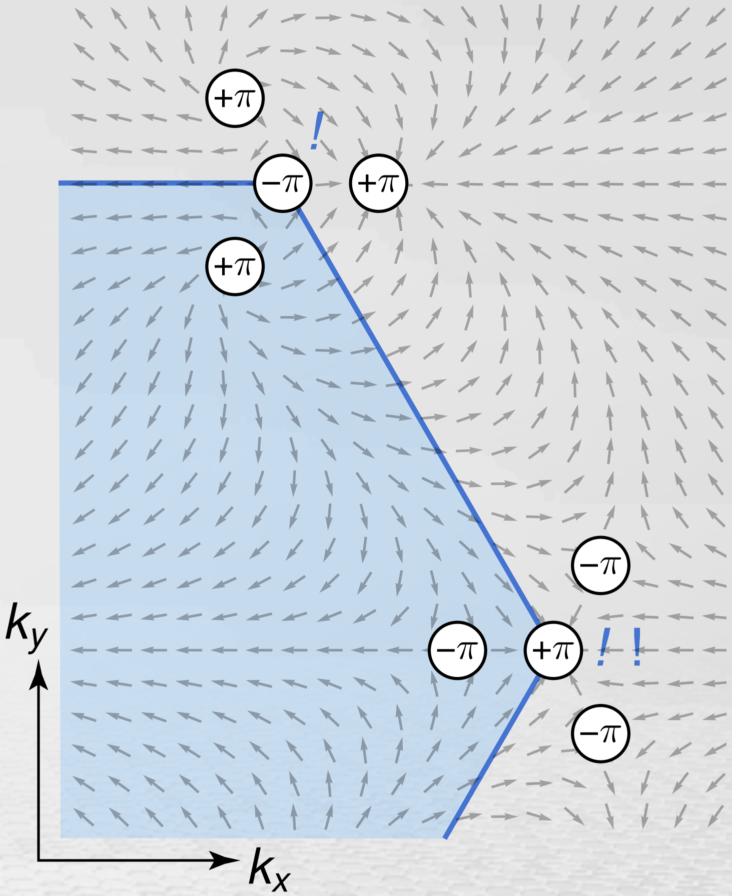


In most implementations violate at least one of the presumably necessary physical properties of *real* Dirac fermions, such as the conservation of chirality, or a local representation.

Certain versions of lattice Dirac fermions preserve the most important properties, but are a technical nightmare, i.e., numerically expensive to work with.

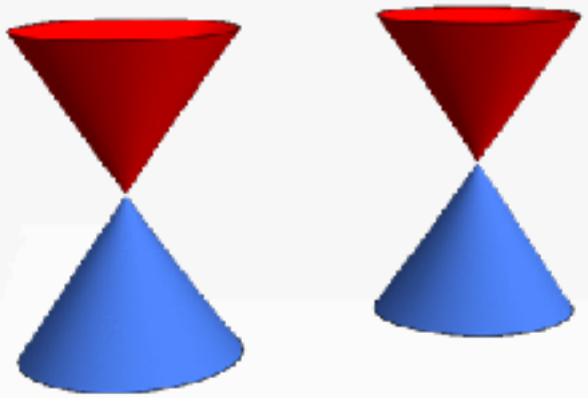
Dirac fermions on the lattice

Recently, new simulations and implementations have been put forward and claim to alleviate known problems of numerical simulations, such as ghost states, fermion doubling and the alteration of universality classes.



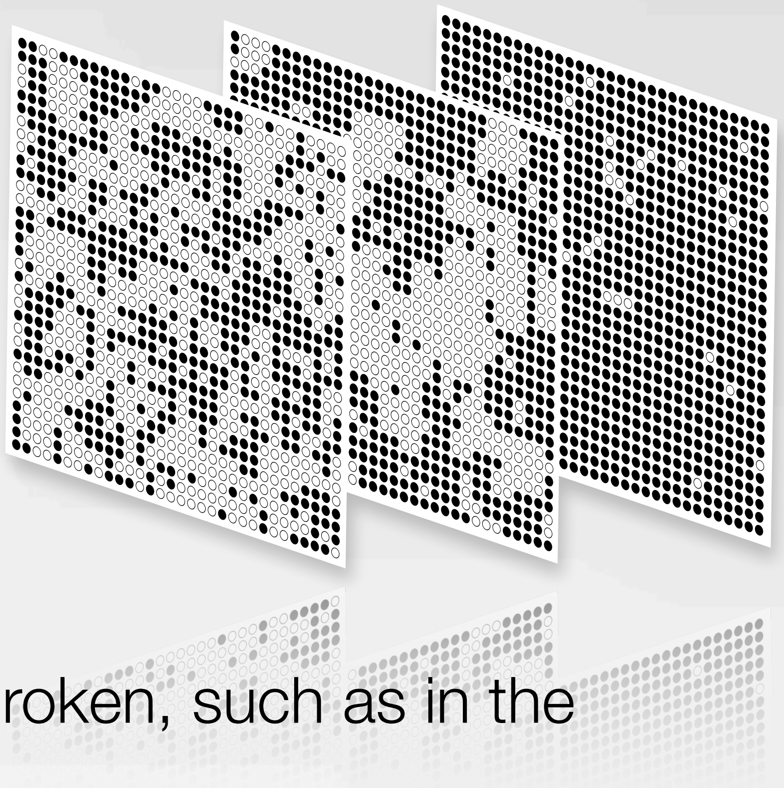
Kronfeld, arXiv:0711.0699 (2007)
T. C. Lang, A. M. Läuchli, Phys. Rev. Lett. **123**, 137602 (2019)
M. J. Pacholski *et al.*, SciPost Phys. **11**, 105 (2021)
A. Donis Vela *et al.*, arXiv:2201.02235 (2022)

The topological properties of these lattice fermions are of particular interest to their application in moire systems, such as twisted multilayer graphene.



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.

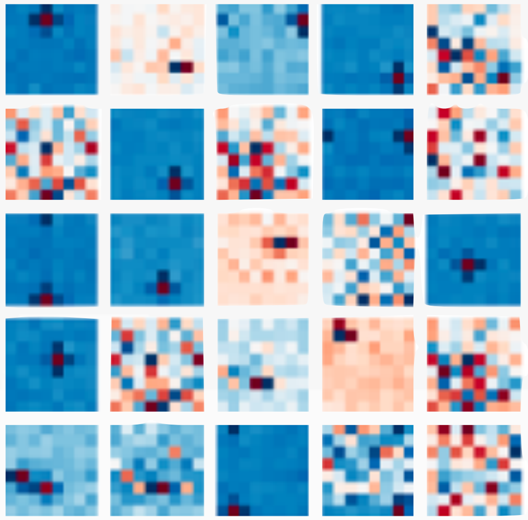
Machine learning, the inverse Ising problem & non-local Monte Carlo updates



Large scale simulations of classical and quantum models have only been made possible by the introduction of non-local (cluster) updates.

No matter how much brute force computing power one invests - you cannot beat a clever algorithm!

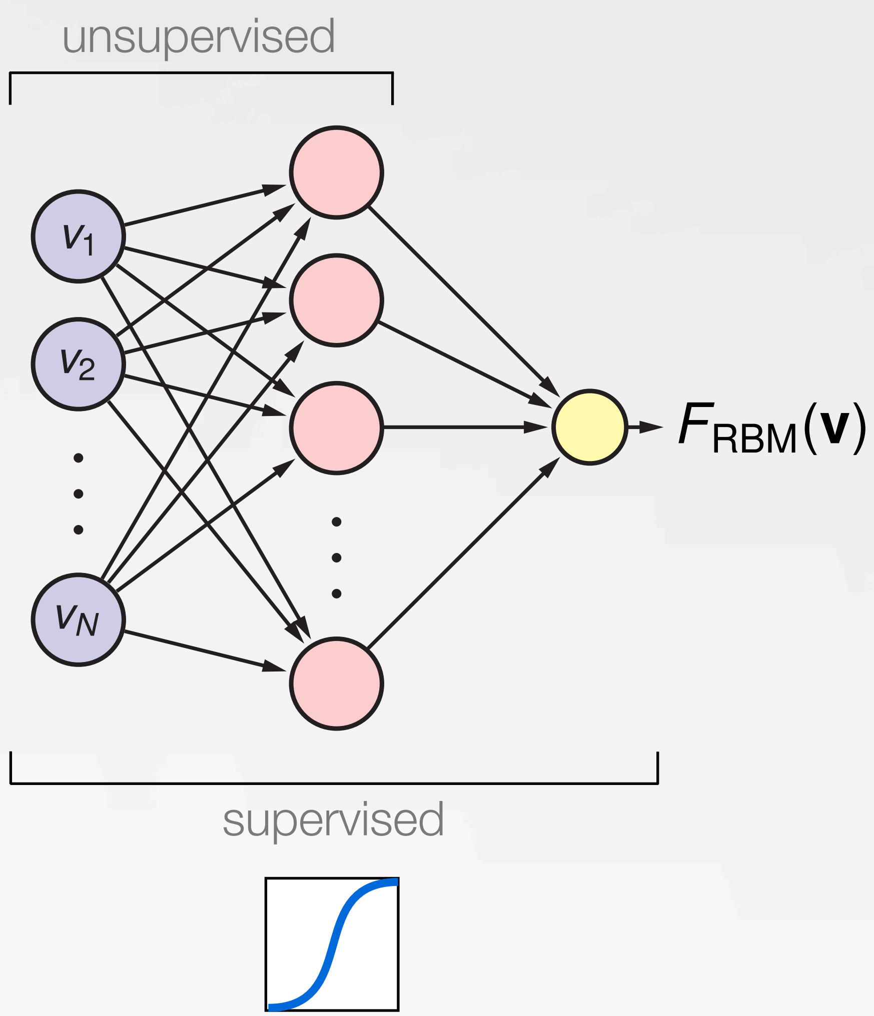
This holds true in particular for simulations close to (quantum) critical points, but also models with complex, or non-local interactions, or systems where symmetries are broken, such as in the presence of external fields.



Non-nocal update algorithms rarely exist, as most of the known ones rely on simple conserved symmetries and simple interactions. Recently, alternatives based on the generation of effective models as sampling basis in Monte Carlo simulations have been proposed.

The applicability of such an algorithm appears promising, but remains unexplored.

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



Alternatively, machine learning introduced the basic neural network, the restricted Boltzmann machine, which allows to be quickly ans inexpensively trained with complex input.

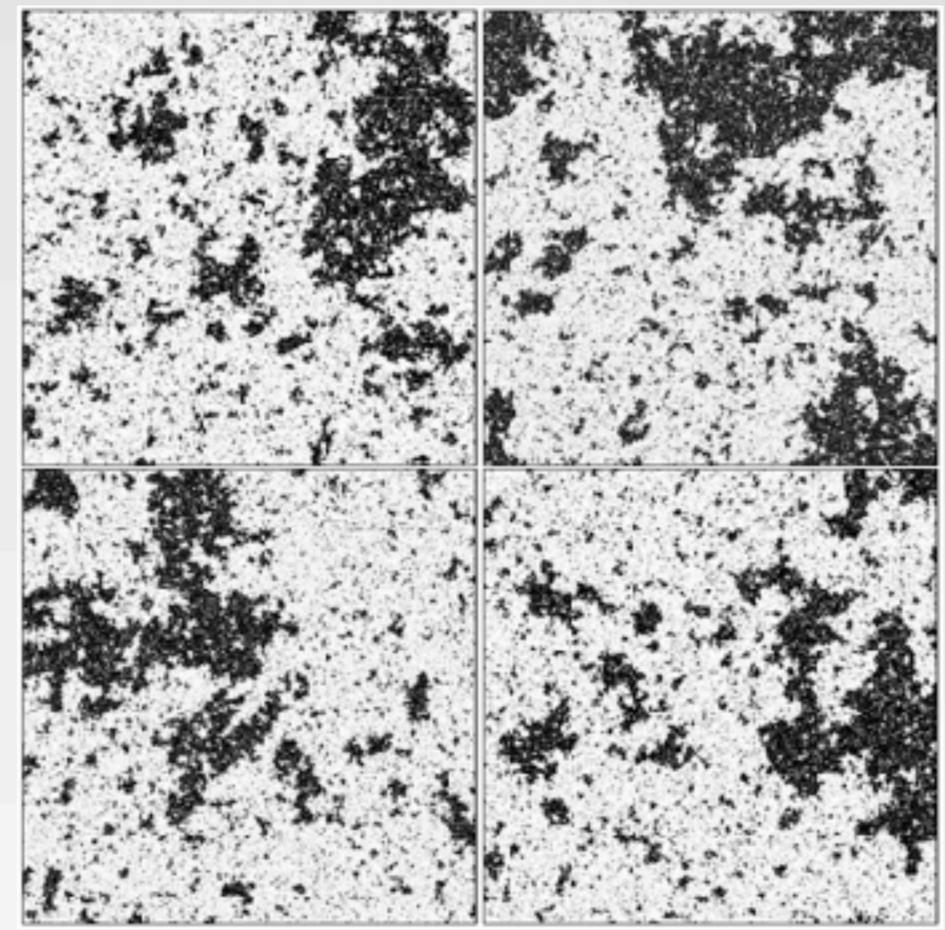
Reversing/activating these trained networks allows to generate configurations suitable for updates in (quantum) Monte Carlo simulations, which are almost exempt from autocorrelations.

L. Wang, Phys. Rev. E **96**, 051301(R) (2017)
L. Huang, L. Wang, Phys. Rev. B **95**, 035105 (2017)
Liu *et al.*, Phys. Rev. B **95**, 041101(R) (2017)

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 RG-invariant

The study of (quantum-) phase transitions and critical theories are at the heart of physics. Investigating phase transitions allows us to unify and classify seemingly disparate physical systems. They represent the junction between phases and as such allow to research the proliferation of excitations, which drive the system into either phase.



By Douglas Ashton

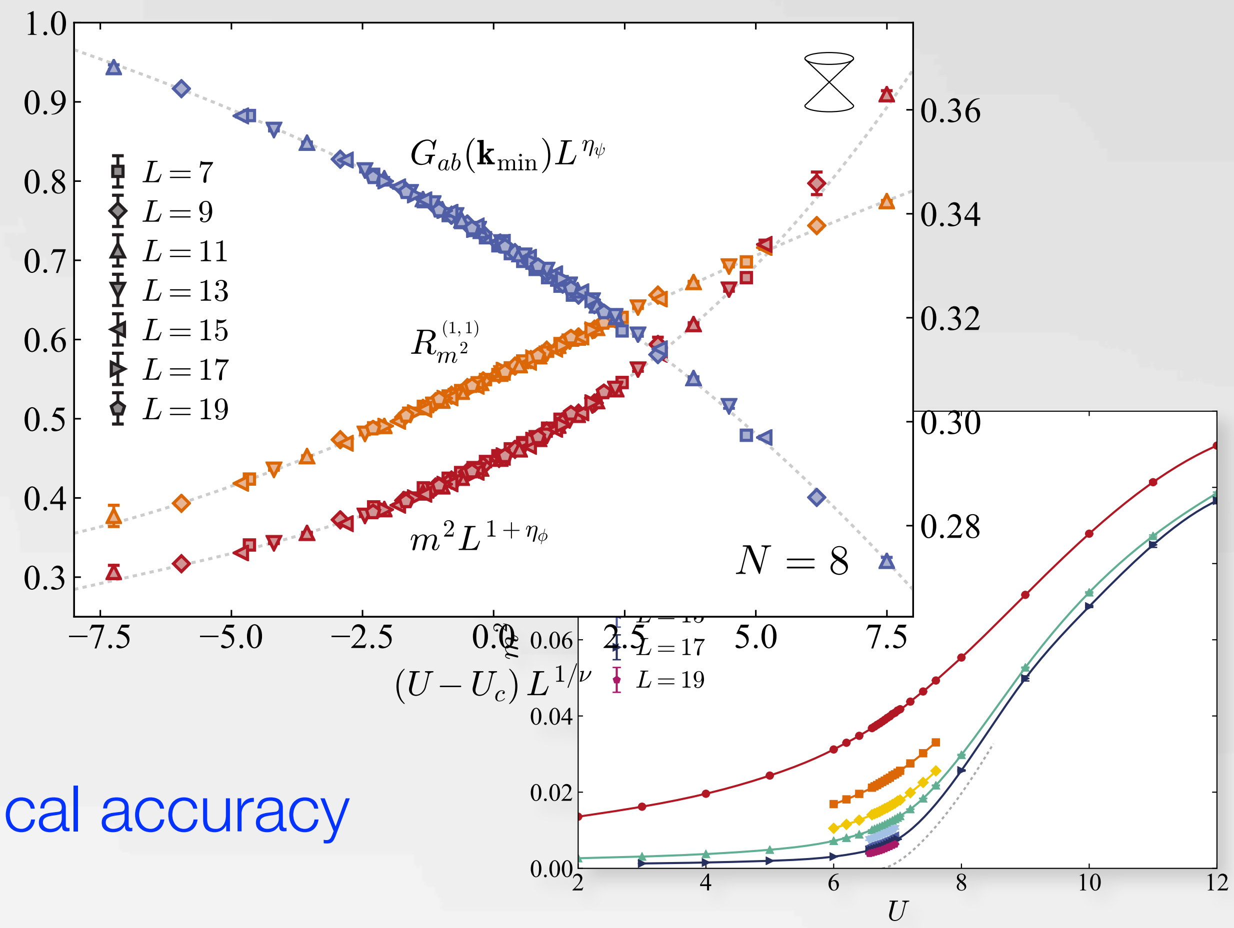
Numerical simulations are restricted to seemingly small finite size systems. Yet, we are interested in the emerging physical properties in the thermodynamic limit, i.e., the macroscopic level.

The finite size scaling ansatz constitutes the most reliable framework to extract critical properties such as the universal exponents at continuous (quantum-) phase transitions from numerical finite size simulations. Based on the concept of scale invariance the physical properties can be cleverly fitted by a scaling function close to criticality.

Finite-Size Scaling at fixed RG-invariant

A newly modified scaling ansatz suggests to expand the scaling function around so called renormalisation group invariant quantities (points).

The numerical analysis is then afflicted by the statistical fluctuations of said quantities rather than those of the usual order parameter.



This yields significant improvement of statistical accuracy as compared to a standard analysis!

F. Parisen Toldin, arXiv:2112.00392 (2021)
M. Campostrini *et al.*, Phys. Rev. B **89**, 094516 (2014)

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.

Contact

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Please don’t hesitate to contact me for details!

- 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

Also, if you already have a certain project, or specific topic in the field of computational condensed matter physics in mind - your suggestions are very welcome!

Programming experience is helpful (in particular for projects 2, 3), but not required!