# Project 1

## Applications of automated symmetry decomposition: quantum chemistry, quantum causality

Subject areas: Quantum Foundations
Supervisor: Denis Rosset

**Project Description:**

Historically, researchers in quantum physics had polarized attitudes towards representation theory. One of the founders of quantum chemistry, John Slater, wrote in the 1920s: "The authors of the 'Gruppenpest' [1] wrote papers which were incomprehensible to those like me who had not studied group theory". Such attitudes persist today in quantum information.

Inspired by recent advances in numerical methods [2], we wrote RepLAB, a MATLAB/Octave toolbox to compute using groups and representations [3]. This toolbox combines symbolical and numerical techniques to approximate key primitives of representation theory. It has two goals: the first one is pedagogical and provides a way for students to play with concrete examples while learning groups and representations. The second one is to speed up computations involving finite dimensional systems with symmetry [4].

The project applies RepLAB to a quantum physics problem to be discussed with the student (ideas below), and will include work on the library itself, for example to optimize concrete computations. Depending on the background/interests of the student (and advances of research at Perimeter!), applications could include:

- Work on quantum causality: How to determine whether observations of a system conform to a particular causal diagram? The same question can be asked for classical and quantum systems. For classical systems, significant contributions to the field of causal inference came from quantum information researchers [5]. Those techniques are extended now to the quantum domain [6]. The computational techniques are expensive, however, the underlying technique (inflation) has internal symmetries begging to be used.

- Systematic study of quantum information resources: quantum information introduced the notion of resources, that is quantum physical systems that have more power than classical systems to perform information tasks (zero knowledge computation, key distribution, etc). A few types of resources have been extensively studied, and only recently an encompassing description has been proposed [7]. However, noise can destroy what makes a quantum resource a useful resource in such tasks. We have algorithms to characterize quantum resources, however, they are CPU expensive. By limiting our study to symmetrical systems, we can push the computational limits.

- Computational quantum chemistry: quantum computers enable the simulation of quantum systems as foreseen by Feynmann. Recently, researchers mapped quantum chemistry problems to quantum hardware on simple molecules [8]. However they did not use symmetries in their encoding. Can we apply automated symmetry decomposition to such problems?

I recommend the student to get in touch with me a few weeks before starting the project so we can tailor the plan.

**Prerequisites:**

Programming skills:

- Prior experience with imperative programming (Fortran/C/Java/Python) a must, then Matlab can be learned easily (we choose Matlab due to the availability of convex solvers + user experience factor).
- Bonus: experience with other paradigms -- functional, data-oriented or quantum programming languages. RepLAB applies some patterns inspired by them.
- The student should be comfortable with object-oriented programming, to the point of working on the library code. Check the source at https://github.com/replab/replab/

Mathematical/physics skills:

- Required: linear algebra, basics of probability theory, introductory quantum mechanics course
- No background in convex optimization expected; student should be comfortable working with https://web.stanford.edu/~boyd/cvxbook/
- No background in group/representation theory is expected; student should be comfortable reading https://link.springer.com/book/10.1007/978-1-4684-9458-7
- Bonus: background in numerical analysis

**References:**

[1] https://ncatlab.org/nlab/show/Gruppenpest
[2] https://link.springer.com/article/10.1007/s13160-010-0007-8
[3] https://replab.github.io/replab/
[4] https://journals.aps.org/prl/abstract/10.1103/PhysRevLett.122.070501
[5] https://www.degruyter.com/view/j/jci.2019.7.issue-2/jci-2017-0020/jci-2017-0020.xml
[6] https://arxiv.org/abs/1909.10519
[7] https://arxiv.org/abs/1909.04065
[8] https://arxiv.org/abs/1907.00362

# Project 2

## Out-of-time-order-correlators as an indicator of chaos?

Subject area: Quantum Information
Supervisors: Alvaro Alhambra and Meenu Kumari

**Project Description:**

Classical chaos - popularly known as butterfly effect - leads to large fluctuations in the evolution of a system due to even very small perturbations. A positive value of the Lyapunov exponent is a well-defined notion of classical chaos, that distinguishes 'chaotic' from 'regular' systems. Due to fundamental differences between classical and quantum mechanics, quantum chaos cannot be defined in the same way as classical chaos. Nevertheless, significant differences have been observed between quantum properties of classically chaotic and classically regular systems, so that we still lack a well-defined characterization of quantum chaos.

Out-of-Time-Order Correlators (OTOCs) were recently proposed as a candidate for a quantum Lyapunov exponent analogous to the classical Lyapunov exponent. OTOCs have begun to be widely recognized as the quantum Lyapunov exponent in the literature, but their validity remains to be rigorously analyzed and proven. For OTOCs to be the correct 'quantum Lyapunov exponent', one would need to show that (a) they are equivalent to the classical Lyapunov exponent for systems that have a well-defined classical limit, and (b) they exhibit distinct behavior for regular and chaotic systems.

To answer these questions, we need to study OTOCs in systems that have a well-defined classical limit, so that they can be compared with the corresponding classical Lyapunov exponent. We propose to study the behavior of OTOCs in a driven simple pendulum (described as 'quantum ratchets" in [1]). This is a relatively simple system that is integrable at zero driving, and can exhibit chaotic behavior upon variations of the driving strength and frequency. This makes it an excellent candidate for the study of OTOCs. Finding a direct correspondence between classical Lyapunov exponent and OTOCs will be a significant step towards understanding the quantum-classical correspondence in chaotic systems, which remains not so well understood yet.

The project will involve both analytical and numerical calculations of the dynamics of this simple system in various parameter regimes, and has the potential for branching out in a few ways if time allows for it. The first step is to solve the Hamilton's equation of motion for the driven simple pendulum numerically and calculate the classical Lyapunov exponent. Then we will numerically solve the time-dependent Schrodinger equation for the driven simple pendulum given an initial quantum state of the system. Finally, we will be able to calculate OTOCs and compare it with the corresponding classical Lyapunov exponent.

Since it is based around a single particle quantum system, we expect that advanced undergraduate students at the level of this program will have most of the necessary background to tackle these questions, which are still timely and relevant for current research. With it, the student will become familiar with the current literature on quantum chaos, and will develop analytical and numerical skills that build directly on their previous training.

**References:**

[1] PRA 75, 063424 (2007).

# Project 3

## Quantum many-body physics on quantum hardware

Subject areas: Quantum Information, Condensed Matter
Supervisor: Timothy Hsieh

**Project Description:**

Recently, there have been significant advances in several quantum computing platforms, including superconducting qubits and trapped ions. At this point, nontrivial quantum operations can be implemented on tens of qubits, and the frontier continues to expand. This project will explore how these emerging technologies can assist the realization and understanding of complex many-body quantum systems, regarding both static aspects such as ground state properties and dynamical aspects such as quantum chaos and thermalization. What new physics can we learn from near-term quantum computers? The ideal outcome is an interesting and realistic proposal that can be carried out in one of the quantum platforms (see for example the interplay between theoretical proposals [1,2] and experiment [3]).

**References:**


[1] W-W. Ho and T. Hsieh, "Efficient Variational Simulation of Non-trivial Quantum States", SciPost Phys. 6, 029 (2019).

[2] J. Wu and T. Hsieh, "Variational Thermal Quantum Simulation via Thermofield Double States", arXiv: 1811.11756 (2018).

[3] D. Zhu, S. Johri, N. Linke, K. Landsman, N. Nguyen, C. Alderete, A. Matsuura, T. Hsieh, and C. Monroe, "Variational Generation of Thermofield Double States and Critical Ground States with a Quantum Computer", arXiv:1906.02699 (2019).

# Project 4

## Range of entanglement in spin chains

Subject area: Condensed Matter
Supervisor: Aaron Szasz

### Project Description:

The transverse field Ising model, the simplest nontrivial quantum spin chain, has a bizarre property: in the ground state, the entanglement between two spins separated by more than two lattice sites is exactly 0.[1, 2] This is true even at the critical point of the model, where the total entanglement across a cut dividing the system in two diverges as the system size goes to infinity; consequently, this total entanglement must come from genuine multipartite entanglement between three or more sites at a time. Because the three-site entanglement is also short-ranged,[3] it appears that multipartite entanglement at all length scales is important, which is quite interesting!

One important question is how generic this short-range entanglement is. Indeed, the same behavior should appear for any model whose ground state does not have long-range order.[4] However, there are still some open questions; here are two promising ones:

1. How does entanglement between two spins fall off with distance in a spin chain with long-range interactions? As the interactions become progressively longer-ranged, there may be a crossover between finite- and infinite-range entanglement; what does that look like?

2. Although entanglement generically is 0 beyond some finite range, the quantum discord, a measure of nonclassicality, is not.[4] A new measure I defined, the accord,[5] lies between these two, so it would be interesting to investigate whether it has finite range like the entanglement or infinite range like the discord.

Working on any or all of these problems will involve first using the density matrix renormalization group (DMRG) method to find the ground states of spin chains, then mixed state entanglement and other quantum correlations like the accord. This project will rely heavily on quantum mechanics and linear algebra, as well as programming in Python. I do not expect familiarity with DMRG, nor with mixed quantum states or entanglement measures, but a student working on this project will learn a lot about all of these topics over the course of the summer. I also do not expect a student to have read any of the papers I cited here; we will start out the project by working through them.

### References:

[1] Phys. Rev. A 66, 032110 (2002).
[2] Nature 416, 608–610 (2002).
[3] Phys. Rev. B 89, 134101 (2014).
[4] Phys. Rev. B 89, 054410 (2014).
[5] Phys. Rev. A 99, 062313 (2019).

# Project 5

## Deconfined Quantum Criticality in a Fermionic System

Subject area: Condensed Matter
Supervisor: Emilie Huffman

**Project Description:**

Strongly correlated quantum many-body systems form an exciting area for theoretical research in many subfields of physics–from condensed matter to nuclear and particle physics. Examples include the structure of nuclear matter such as the quark-gluon plasma, strongly-correlated materials such as high Tc superconductors, strange metals and frustrated magnets, unitary atomic gases, and even speculative physics beyond the standard model and quantum gravity. A single model can often be applicable to a few of these disparate fields at once. In the strongly correlated regime, relatively simple quantum many-body Hamiltonians can possess remarkably rich phase diagrams with second order quantum phase transitions between the different phases. These transitions are characterized by critical exponents--which are the same for different microscopic models that fall within the same universality class and are determined by certain key symmetries. Since second order transitions are governed by correlations among many degrees of freedom, quantitative predictions are difficult–using analytic methods and high performance comping becomes necessary. Here I propose a project for studying quantum critical phenomena in a specific strongly correlated lattice fermionic system and extracting its universal properties using quantum Monte Carlo (QMC) methods.

We would be looking at a fermionic model with a four-fermi interaction that has the same key symmetries as the model studied in Ref. [1] with QMC. It has been proposed to have an exotic deconfined quantum phase transition (DQCP) with emergent SO(5) symmetry and critical exponent \eta = 0.59, however only lattices with up to 800 sites were used in this calculation, and finite size effects are an important consideration when working on the lattice. This fermionic result is in seeming contradiction with critical exponent calculations for spin systems in the past that involved the same key symmetries and are thought to be in the same universality class. Additionally this new \eta value is just barely over the bootstrap minimum requirement of \eta=0.52 in order to have a DQCP. While there have been multiple studies of the spin models, there has only been one for the fermionic model and so more study is warranted. I have developed fermionic algorithms that are able to study fermionic systems much larger than were reachable for traditional auxiliary field methods, as used in the previous study of this model. The only major difference between this DQCP-candidate model and the model I have studied before is the number of flavors.

The goal would thus be for us to look at this model and take these calculations to over twice the number of fermionic sites (48^2= 2304 sites with \beta= 48.0) compared to before to see if finite-size effects are still a factor for the fermions. We will be able to determine with more confidence whether the transition is truly second-order, and if so, what its critical exponents are, and if they are indeed over the bootstrap minimum still. Because the base of this code is already written, the student would be able to work on adding a few model-specific modifications to it (such as writing new observables) as well as exploring different parameters in order to find the critical region for this model. They would also get experience running QMC calculations on supercomputing resources, and learn the physics necessary to extract critical exponents from the data. They would gain a lot of experience with the study of strongly interacting many-body fermionic systems.

**References:**


[1] arXiv:1904.10975

# Project 6

## Prospects for uncovering new physics with future cosmological surveys

Subject area: Cosmology
Supervisors: Junwu Huang, Moritz Münchmeyer, and Davide Racco

### Project Description:

A great deal of information about the physics governing the early Universe can be extracted from the measurement of correlation functions of CMB and large-scale structure in the cosmos. The most exciting prospects from the perspective of particle physics is to detect the effects of massive particles at high energy scales far beyond those accessible by particle accelerators. Recently theorist have developed a more detailed understanding of such signatures, but it is not fully understood to what extent they could be visible in present or upcoming cosmological data. In this project, we will make simple forecasts for constraints or detections with cosmological surveys. In the next years, CMB experiments and galaxy surveys will be the most powerful methods. In the long term, a particularly promising frontier is intensity mapping of the distribution of neutral hydrogen in the universe, which could revolutionize our knowledge of inflationary particle physics.

The project touches both cosmology and particle theory. On the cosmology side, we will develop a forecast in the spirit of [1] (co-authored by Moritz Münchmeyer) but for different data sources and with new theoretical signatures. On the theoretical side, the student will learn about high energy scenarios which could be probed through the measurement of distinctive signatures in correlation functions. As a specific case study, we will apply these techniques to the scenarios studied in [2] and [3] (co-authored by Junwu Huang and Davide Racco), where the origin of the signal lies within the Standard Model of particle physics, with basically no assumption about unknown physics.

### References:

[1] arXiv:1610.06559
[2] arXiv:1907.10624
[3] arXiv:1908.00019

# Project 7

## Cross-correlation between stochastic gravitational wave background and other cosmological backgrounds

Subject area: Cosmology
Supervisor: Ghazal Geshnizjani

**Project Description:**

Gravitational waves (GWs) are one of the striking predictions of the General Theory of Relativity. The first direct detection of GW signals emitted from a merging black hole pair in 2015, has started a new era in astronomy and cosmology. They potentially contain information about cosmological sources, which would be otherwise not possible to extract through electromagnetic signals. However, all the GW signals observed so far have been emitted from bright sources resolved as distinct events, such as low-redshift black hole and neutron star binary mergers. In principle, one expects that there are additional information buried in the gravitational wave stochastic background emitted from sources, which are either too far away or too faint to be detected individually. In particular, inflations and other phenomena in early universe would fall into this category. In this project, we will study cross-correlation between this stochastic GWB and other cosmological backgrounds such as galaxy surveys to extract information about earlier phases of universe.

# Project 8

## Galaxy cluster masses with convolutional neural networks

Subject area: Cosmology
Supervisor: Mathew Madhavacheril

**Project Description:**

Weighing massive galaxy clusters is a central goal of cosmological projects aimed at constraining properties of the universe, including understanding the origin of dark energy. Galaxy clusters are dominated by dark matter making their masses very difficult to measure based on just the light they emit. However, background sources of light are bent or 'lensed' by the gravitational influence of the cluster, and this lensing effect can help us infer the mass of the lensing cluster. In particular, light from the cosmic microwave background (CMB) can be used to measure the mass of any galaxy cluster since the CMB is the farthest back our telescopes can pick up photons from.

Current methods for measuring galaxy cluster masses from the CMB are somewhat noisy since they were originally meant to measure the lensing effect due to very large-scale structures. More recently proposed "maximum likelihood" methods are however more susceptible to contamination from "foregrounds" like emission from dust. In this project, we will explore the possibility of estimating masses using convolutional neural networks (CNNs) that are trained using simulated lensed CMB images.

The primary challenge with such an application of CNNs is model bias -- the possibility that a mismatch between the simulated foregrounds and the observed foregrounds can cause the inferred masses to be wrong. To address this, we will explore an extension of CNNs wherein the training set image consists of not just the input lensed image but also a modified copy of the image that retains only the large scale background gradient in the image. Since lensing (unlike foregrounds) has the unique property of correlating the small-scale fluctuations in the map with the large scale background gradient of the image, this method could allow the network to learn that correlation more robustly, allowing for foreground-bias-free inference of galaxy cluster masses.

**Prerequisites:**

- Introductory astronomy/cosmology is useful
- Some exposure to coding in Python (or Matlab or R or similar) is highly recommended

# Project 9

## Sparse Grids

Subject areas: Strong Gravity, Computational Physics
Supervisor: Erik Schnetter

### Project Description:

It is today not yet possible to solve high-dimensional partial differential equations with numerical methods. For example, studying neutrino transport in neutron stars or the dark matter halo of galaxies requires solving equations in 7 dimensions (3 space, 3 momentum, 1 time), and currently used discretization methods are too expensive in this case, even on the world's largest supercomputers.

Sparse Grids [1] may provide a way out. Sparse Grids represent high-dimensional manifolds in a provably optimal way that might make such systems solvable even on a single computer [2]. The aim of this project is to learn about sparse grids, to apply them to solving the Vlasov equation e.g. to study dark matter halos of galaxies, and to extend and improve the method as necessary.

### Required skills:

- Linear algebra sufficient to read [1] and [2]
- Programming, preferable in Julia

### References:


[1] https://pdfs.semanticscholar.org/9367/0b2257d60c866a6d32ad864f2eb640fe26f0.pdf
[2] https://arxiv.org/abs/1710.09356