# Intern projects

Jason Kaye

**Numerical methods for the nonequilibrium Dyson equation**

The use of the Keldysh approach in the simulation of quantum many-body dynamics out of equilibrium has grown in popularity over the last several years. It requires solving a collection of nonlinear Volterra integro-differential equations, referred to as the nonequilibrium Dyson equations (NDE), for the various Keldysh components of the many-body Green's function. One of the primary computational bottlenecks in solving the NDE stems from memory effects taking the form of history integrals, which lead to a naive cubic scaling with the number of time steps. This limits practical simulations to short times, and represents a significant limitation of the Keldysh method. However, recent efforts involving linear algebraic compression methods have led to a reduced scaling for a wide class of problems, suggesting a path towards solvers capable of reaching very large propagation times.

The project will continue this research effort, focusing on one of several possible related research topics depending on the interest of the intern. These include (1) the performance of global iterative solvers vs. solvers based on time stepping, (2) the advantages and disadvantages of alternative formulations of the NDE, (3) the combination of compression methods with high-order adaptive time stepping, and (4) the application of our solvers to specific problems in nonequilibrium quantum physics. Since we will likely focus primarily on algorithm development, this project would be a good fit for an individual with a strong interest in numerical methods for scientific computing and/or applied mathematics. For interns with a background in software development, the project could also focus on the development of codes for use by the larger computational physics community.

References

J. Kaye, D. Golez. "Low rank compression in the numerical solution of the nonequilibrium Dyson equation," SciPost Phys. 10, 091 (2021).

M. Schuler, D. Golez, Y. Murakami, N. Bittner, A. Herrmann, H. U. R. Strand, P. Werner, M. Eckstein. "NESSi: The Non-Equilibrium Systems Simulation package," Comput. Phys. Commun. 257, 107484 (2020).

F. Meirinhos, M. Kajan, J. Kroha, T. Bode. "Adaptive numerical solution of Kadanoff-Baym equations," SciPost Phys. Core 5, 030 (2022).

Sophie Beck and Andrew Millis

**Di and Tri-halides: a new class of quantum materials**

The transition metal di- and trihalides (materials such as VI3 and RuCl3) form in layered triangular and Kagome structures and display a wide and still not fully explored range of correlated electron behavior, including Mott and charge transfer insulating states, magnetism and interesting spin liquid phases. They can be synthesized in different forms, including in monolayer, multilayer and bulk, and can be exfoliated, stacked and twisted. The series of compounds that can be synthesized is in some ways analogous to the familiar pseudocubic pervoskite family, but the two-dimensionality and different symmetry (D3d or D6 rather than Oh and its derivatives) may lead to different physics, including spontaneously generated one-dimensional structures and also phases with topological content.

In this project we propose to use beyond DFT methods, especially the DFT+DMFT+c-RPA suite of tools, to survey the many-body electronic structure of this family of materials, identifying phases and phase transitions, and, in a potential second phase of the project, to identify a small number of compounds for further intensive study. The project will be in collaboration with Sophie Beck and Andrew Millis, and others at CCQ. Ongoing collaborations with experimental groups at Columbia and the University of Washington may lead to opportunities to model and understand experimental data.

Fabijan Pavosevic, Angel Rubio and Johannes Flick

**Making Polaritonic Coupled Cluster Machine Learnable**

Among various approaches, the polaritonic quantum electrodynamics coupled cluster (QED-CC) method [1-2] offers a systematic way for describing the processes inside an optical cavity by treating electrons and photons quantum mechanically on the equal footing. However, its applicability is hampered by the steep computational cost. The aim of this project is to develop a computationally efficient yet accurate alternative to the QED-CC method. In particular, in this project we will focus on development of the electron-photon exchange correlation functional using machine learning techniques. This will be achieved by rewriting the QED-CC energy expressions in terms of energy density which in turn depends on the molecular grid [3]. As written in this form, we will inspect dependence of the energy density as a function of electron density. Using the symbolic regression, we will construct an accurate functional in the symbolic form that approximate a dataset [4]. Finally, the developed functional will be employed to study pericyclic reactions under the strong-light matter regime. The expected outcome of this project is to develop an electron-photon exchange correlation functional for accurate treatment of molecular polaritons. This project will make you familiar with high-performance computing systems, the python software language, machine-learning concepts, quantum chemistry, and physical organic chemistry.

1. Haugland, T. S., Ronca, E., Kjønstad, E. F., Rubio, A., Koch, H. (2020). Coupled cluster theory for molecular polaritons: Changing ground and excited states. *Physical Review X*, *10*(4), 041043.
2. Pavošević, F., Flick, J. (2021). Polaritonic unitary coupled cluster for quantum computations. *Journal of Physical Chemistry Letters 12*, 9100.
3. Margraf, J. T., Kunkel, C., Reuter, K. (2019). Towards density functional approximations from coupled cluster correlation energy densities. *The Journal of Chemical Physics*, *150*(24), 244116.
4. Ma, H., Narayanaswamy, A., Riley, P., & Li, L. (2022). Evolving symbolic density functionals. *Science Advance, 8(36)*

Olivier Gingras, Sophie Beck, and Antoine Georges

**The role of angle rotations in the magnetic state of Sr3OsO6**

Experimental measurements of the magnetization in thick-film cubic Sr3OsO6 have suggested high-temperature ferromagnetism above 1000 K [1], while bulk non-cubic measurements do not [2]. Our one-shot DFT+DMFT calculations instead predicted an antiferromagnetic transition around 150 K in the cubic phase, along with the absence of magnetism down to low temperature for the non-cubic one [3]. The repression of magnetism was attributed to the tilt and rotations of the octahedron cage of oxygen surrounding the osmium atom [3]. In this project, we propose to study these effects by simulating the extrapolated structure between the cubic and non-cubic symmetries using DFT+DMFT. The effect of doping could also be studied.

[1] Y. K. Wakabayashi *et al.*, Ferromagnetism above 1000 K in a highly cation-ordered double-perovskite insulator Sr3OsO6, *Nature communications* **10**, 1 (2019).
[2] J. Chen *et al.*, Study of polycrystalline bulk Sr3OsO6 double-perovskite insulator: comparison with 1000 K ferromagnetic epitaxial films, *Inorganic Chemistry* **59**, 4049 (2020).
[3] O. Gingras, S. Beck, L. V. Pourovskii, O. Parcollet and A. Georges, *in preparation*.
[4] S. Das *et al.*, Understanding the curious magnetic state of Sr3OsO6, *Physical Review B* **101**, 184422
(2020).

Kun Chen

**Feynman Diagram Compiler based on Computational Graph**

Feynman diagram is a common language of modern quantum many-body theory. It gives a vivid visualization of the mathematical expressions describing the behavior and interaction of quantum particles. As the order of interactions increases, the number of Feynman diagrams

factorially grows, making them challenging to enumerate. We recently found that the computational graph technique that powers the machine learning community provides a compact representation of high-order Feynman diagrams. Based on this idea, we are developing a mini-compiler to generate and calculate Feynman diagrams (https://github.com/numericalEFT/FeynmanDiagram.jl). Although in an early stage of development, this tool is already helping solve problems in many research facilities worldwide. We invite intern candidates to help us to create new frontends for new kinds of Feynman diagrams, invent new algorithms for automatic differentiation and integration, or use the tool to explore new applications in quantum many-body systems.

**Andrew Millis**

**Dynamical Mean Field Theory of Twisted Bilayer Graphene**

'Moire' materials made of two or more atomically thin layers stacked at a small twist angle have revealed remarkable new physics, including exotic Chern Insulator and valley coherent states, and superconductivity. Recent experimental work has revealed novel intermediate-temperature physics including high entropy metallic states and `Pomeranchuk'-like entropy stabilized phase transitions [1] which cannot easily be studied by the Hartree-Fock and wave functions methods in current wide use. In this project, we will use a new Wannier representation of the materials [2] and state of the art dynamical mean field theory to calculate the phase diagram at non-zero temperature and figure out the entropic effects.

[1] Entropic evidence for a Pomeranchuk effect in magic angle graphene arXiv:2009.01836

[2] Real space representation of topological system: twisted bilayer graphene as an example arXiv:2210.11573