Intern projects 2024

Jason Kaye and Dominik Kiese

Compressed representations of n-particle correlation functions and vertex functions

The exploration of strong electronic correlations in real materials is one of the great frontiers of condensed matter physics research. Theoretically, local correlations can be non-perturbatively incorporated using single-site dynamical mean-field theory (a self-consistent description of a single atom coupled to a bath). In order to describe non-local fluctuations, as relevant for emergent phenomena like superconductivity and quantum criticality, however, one needs to go beyond single-site calculations. A crucial ingredient for computing, e.g. the response of a material to small external perturbations, are n-particle vertex functions. The 2-particle vertex in the spin channel, for example, can be used to calculate the magnetic susceptibility, a key observable for probing long-range magnetic order.

Significant progress has recently been made on the efficient representation and manipulation of single-particle correlation functions, and related quantities such as the electronic self-energy, in the imaginary time and Matsubara frequency domains [1,2]. This has relied on low-rank compression of the subspace containing these functions, which are universally characterized by a spectral representation. Significant open problems remain in generalizing these ideas to two-particle and n-particle correlation functions, as well as vertex functions, in a manner amenable to practical calculations. These include (i) the identification of relevant spectral representations, (ii) the development of efficient methods of obtaining compressed representations of functions from their samples, and (iii) the development of fast algorithms to perform diagrammatic calculations using these compressed representations. This project will continue ongoing work in CCQ to develop robust tools and software for vertex calculations in parameter regimes well beyond those accessible today.

[1] J. Kaye, K. Chen, O. Parcollet, "Discrete Lehmann representation of imaginary time Green's functions", Phys. Rev. B, 105, 235115 (2022).
[2] H. Shinaoka, J. Otsuki, M. Ohzeki, and K. Yoshimi, "Compressing Green's function using intermediate representation between imaginary-time and real-frequency domains," Phys. Rev. B, 96 (3), 035147 (2017).
[3] M. Wallerberger, H. Shinaoka, A. Kauch, "Solving the Bethe-Salpeter equation with exponential convergence," Phys. Rev. Research, 3 (3), 033168 (2021).

Jason Kaye and Sophie Beck

Development and application of efficient algorithms for Brillouin zone integration

Brillouin zone (BZ) integration is a standard operation in electronic structure calculations for crystalline solids, required to compute physical observables such as the density of states and the optical conductivity. Substantial recent progress has been made in designing efficient and robust integration algorithms which take advantage of the special structure of the BZ and the integrands appearing in typical calculations, including adaptive methods [1,2] and methods based on complex analysis [3]. The use of these algorithms in large-scale codes promises to offer significantly more reliable results in extreme parameter regimes which were previously out of reach.

Depending on the interests of the intern, this project can focus on (i) further research into advanced BZ integration algorithms, (ii) applications of adaptive BZ algorithms which have been developed in CCQ to problems in many-body physics, or (iii) implementation of these algorithms in codes developed at CCQ. For (i), we are primarily interested in exploring complex-analysis based techniques to push further into the difficult regimes of very low temperatures, very small electron scattering rates, and a large number of electronic bands. For (ii), the aim is to explore various applications of advanced integration algorithms within the density functional theory + dynamical mean-field theory framework applied to strongly correlated materials, in particular at low temperature. Possible examples include the limited accuracy in impurity solvers due to coarse BZ sampling or the calculation of post-processing observables with unprecedented resolution.

[1] J. Kaye, S. Beck, A. Barnett, L. Van Muñoz, O. Parcollet, "Automatic, high-order, and adaptive algorithms for Brillouin zone integration", SciPost Phys., 15 (2), 062 (2023).
[2] E. Assmann, P. Wissgott, J. Kuneš, A. Toschi, P. Blaha, K. Held, "woptic: Optical conductivity with Wannier functions and adaptive k-mesh refinement", Comput. Phys. Commun. 202, 1 (2016).
[3] I. Duchemin, L. Genovese, E. Letournel, A. Levitt, S. Ruget, "Efficient extraction of resonant states in systems with defects", J. Comput. Phys., 477, 111928 (2023).

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.

Leo Cunha, Angel Rubio and Johannes Flick

Extending the Polaritonic Chemistry Toolbox Beyond Energetics: method development and benchmarking molecular properties in cavities

Recent advances in optical confinement at the nanoscale have led to a renewed interest in leveraging strong light-matter coupling to control the properties of molecules and materials. Theoretically, extensions of traditional electronic structure methods, such as coupled-cluster theory (QED-CC) [1,2] and density functional theory (QEDFT) [3,4,5], have been proposed to treat light and matter degrees of freedom on equal footing in the polaritonic regime. While most of the recent studies have solely focused on energetics, understanding how properties are modulated by the optical cavities are of paramount importance to achieve control over chemical processes. Possible internship projects in the polaritonic's team are listed below:

1. Understanding how optical cavities contribute to structural modifications, such as equilibrium geometries and harmonic frequencies, in molecular polaritons.
2. Investigating how polaritons can modulate band structure of materials.
3. Analyzing how different photonic observables change in the course of a chemical reaction.

For each of the topics above, interns will have the opportunity to run polaritonic simulations using in-house QED-CC and QEDFT codes, compare the performance of different levels of approximation and benchmark chemical properties inside optical cavities. At the end of the program, interns will have gained experience and expanded their background in quantum chemistry, programming in python and high-performance computing systems.

1. Haugland, T. S. *et al.*, "Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States", ***Phys. Rev. X***, 10, 041043 (2020).

2. Pavošević, F. *et al.*, "Cavity-Modulated Proton Transfer Reactions", ***J. Am. Chem. Soc.***, 144, 11, 4995–5002 (2022).
3. Ruggenthaler, M. et al., "Quantum-electrodynamical density-functional theory: Bridging quantum optics and electronic-structure theory", ***Phys. Rev. A***, 90, 012508 (2014).
4. Schäfer, C. *et al.,* "Making ab initio QED functional(s): Nonperturbative and photon-free effective frameworks for strong light–matter coupling", ***Proc. Natl. Acad. Sci.,*** 118.41, e2110464118 (2021).
5. Flick, J., "Simple Exchange-Correlation Energy Functionals for Strongly Coupled Light-Matter Systems Based on the Fluctuation-Dissipation Theorem", ***Phys. Rev. Lett.***, 129, 143201 (2022).

Paul Yang

Explore spin and charge orders in TMD heterobilayers

Strongly interacting electronic phases are being discovered at an astonishing pace in moiré materials. In the past three years, generalized Wigner crystal (GWC), fractional Chern insulator (FCI), Kondo heavy fermion and kinetic magnetism have all been realized in transition metal dichalcogenide (TMD) bilayer devices. Fundamentally semiconductor junctions, these devices host confined electrons, which are well-described by the two-dimensional electron gas (2DEG) model.

In this project, we will use density functional theory (DFT) and other methods to solve the 2DEG model in an external moire potential and explore the charge and magnetic orders that arise.