Many-Body Electronic Structure Calculations for Solids

Lausanne, March 11^{th} - March 13^{th} 2024

Book of Abstracts

Antoine Levitt (Université Paris-Saclay)
Title: Numerical methods for Brillouin zone integration.
Abstract: In the framework of mean-field methods such as DFT, the periodicity of solids can be exploited using Bloch's theorem, reducing the computation of the electronic structure of a solid to unit cell problems, parametrized by a quasi-momentum variable belonging to the Brillouin zone. Quantities of interest are then expressed as integrals over the Brillouin zone. To compute them numerically, integration schemes have to be used. I will review the different schemes used, and discuss a recently proposed method to use a complex deformation of the Brillouin zone to speed up the integration.

Andre Laestadius (Oslo Metropolitan University)
Title: The use of Moreau-Yosida regularization in density-functional theory.
Abstract: The universal density functional in density-functional theory (DFT) is not regular (it is everywhere discontinuous in the standard formulation). In this talk, I will discuss the use of the Moreau-Yosida regularization in density-functional theory. Specifically, we will examine the role of Moreau-Yosida regularization for the inverse problem of DFT: given the ground-state density of an interacting quantum system, how can we determine an effective potential that can produce the same density for some 'simpler' Hamiltonian?

Mi-Song Dupuy (Sorbonne Université)
Title: An overview of one-dimensional area law in DMRG.
Abstract: The Density Matrix Renormalisation Group (DMRG) is a widely-used numerical algorithm for computing low-energy eigenstates of Hamiltonians with local interactions. A key aspect of its effectiveness was elucidated by Hastings, who showed that ground-states of one-dimensional nearest neighbor interaction Hamiltonians follow an area law. This means that the block entropy of the ground-state projector depends on the surface area of the block rather than its volume, a consequence of the ground-state's amenability to low-rank approximation via tensor trains or matrix product states. In this talk, we provide an overview of two main proof strategies: Hastings' original approach, which relies on the Lieb-Robinson bound, and the Approximate Ground-State Projector (AGSP) method introduced by Arad et al.

Örs Legeza (Wigner Research Centre for Physics)
Title: Mode optimized restricted active space density matrix renormalization group method for electronic structure calculations on high performance computing infrastructures.

Andreas Grüneis (Technische Universität Wien)
Title: Periodic coupled cluster theory applied to condensed matter and surface chemistry problems.

Fabian Faulstich (Rensselaer Polytechnic Institute)
Title: On a recent coupled cluster theory based static quantum embedding scheme.
Abstract: I present a static quantum embedding scheme that utilizes projection equations to solve coupled cluster amplitudes. To reduce computational costs, the presented procedure solves the local fragment problem using a high-level coupled cluster method whereas the environment problem is solved with a lower-level perturbative method. This embedding approach is consistently formulated within the coupled cluster framework. We demonstrate the effectiveness of our method through several prototypical molecular examples using both small and large basis sets. The accuracy of our method can be comparable to that of applying the high-level method to the entire system. Additionally, our results indicate that increasing the fragment size can systematically enhance the accuracy of observables, approaching the precision of the full coupled cluster solver.

Reinhold Schneider (Technische Universität Berlin)
Title: Wavelet Analysis for Periodic Coupled Cluster.
Abstract: Periodic electron structure theory is mainly based on Floquet Bloch theory. In contrast to DFT (density functional theory, wave function approximations for periodic systems suffer from extremely bad scaling w.r.t. the number N_k of k-points, which is e.g. $\mathcal{O}(n^4 N_k^3)$ for storage and $\mathcal{O}(n^6 N_k^5)$ for computational cost. We consider the Coupled Cluster CC(S)D approximation for periodic systems and ground state calculation for insulating systems. After investigating the singularity structure of the electron repulsion integral snd the CCD amplitudes, we introduce an adaptive wavelet representation. Theoretically, complexity of this representation can be reduced to almost linear scaling w.r.t. to N_k.

Thomas Bondo Pedersen (University of Oslo)
Title: TBA.
Abstract: TBA.

Eva Pavarini (Forschungszentrum Jülich)
Title: Strongly-Correlated Materials: the Dynamical Mean-Field Theory Perspective.
Abstract: Strongly-correlated systems are characterized by emergent cooperative phenomena that escape the static mean-field description. Their discovery is in most case experimentally driven, and gives typically rise to decades of intense investigations and hot debates. Paradigmatic examples are the Mott transition, orbital ordering, and non-conventional superconductivity. A major theoretical breakthrough for the description of classes of these phenomena was the dynamical mean-field theory (DMFT) and its combination with density-functional theory-based methods –the so-called DFT+DMFT technique. In this talk I will introduce the approach, discuss the theoretical state of the art and open problems, and present paradigmatic applications.

Benjamin Stamm (Universität Stuttgart)
Title: Reduced basis surrogates for quantum spin systems based on tensor networks.
Abstract: In this talk, we present a reduced basis method for quantum spin problems. Within the reduced basis methods approach, an effective low-dimensional subspace of a quantum many-body Hilbert space is constructed to investigate, e.g., the ground-state phase diagram. The basis of this subspace is built from solutions of snapshots, i.e., ground states corresponding to particular and well-chosen parameter values. Here, we show how a greedy strategy to assemble the reduced basis and thus select the parameter points can be implemented based on matrix-product-states (MPS) calculations using DMRG optimization. Once the reduced basis has been obtained, observables required for the computation of phase diagrams can be computed with a computational complexity independent of the underlying Hilbert space for any parameter value. We illustrate the efficiency and accuracy of this approach for different one-dimensional quantum spin-1 models and study empirically the Kolmogorov width for increasing chains.