Theoretical spectroscopy with ab initio Green's function-based methods

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Green's function-based many-body perturbation theory (MBPT) is a state-of-the-art approach for calculating charged and neutral excitations in condensed matter systems. In particular, the GW approach and the Bethe-Salpeter Equation have been used widely for predicting optoelectronic properties of bulk and nanostructured materials. Due to significant advancements in software and hardware development, these methods can nowadays be applied to complex materials with hundreds of atoms, allowing for predictive theoretical spectroscopy that aids in interpreting experiments, developing physical insight, and predicting new materials and properties.

The goal of my presentations and hands-on exercises during this Summer School is to provide an accessible entrance into the world of MBPT with a focus on the GW and Bethe-Salpeter Equation approaches. We will start with a short introduction into density functional theory (DFT) – a foundational, and in-principle exact, method for calculating ground-state properties. We use DFT to calculate single-particle energies and orbitals that serve as zeroth-order starting points for MBPT. I will then explain the main rationale behind the GW and Bethe-Salpeter Equation approaches, highlighting common approximations, their strengths and limitations, and show some pertinent applications of these methods in condensed matter physics. Additionally, we will work on a series of hands-on exercises that will allow the students to learn how these methods work in practice and obtain experience with their implementation in the open-source codes Quantum Espresso and BerkeleyGW.