Predictive algorithms for simulating quantum materials (Quantum Algorithms)
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This project seeks to advance the field of predictive algorithms for quantum many-body systems by developing a next-generation numerical toolset. The project will focus on combining field-theory based methods for both perturbative and non-perturbative ab-initio and model systems with innovations in tensor techniques, quantum Monte Carlo, machine learning, and numerical analysis. By utilizing these innovative methods, we aim to deepen our understanding of quantum phases and exotic properties of materials, focusing in particular on experimentally measurable quantities. Currently, accurate methods for studying correlated quantum materials and their excitations are lacking. Established technology either employs the so-called density functional theory, which relies on uncontrolled approximations to electron correlations and may be imprecise for systems with partially filled d- or f-shells, or proceeds by downfolding to an effective low-energy model which may capture correlations but neglects import aspects of electronic structure. Recent years have seen substantial progress in methodologies for simulating finite-temperature field theories ab-initio, using diagrammatic perturbation theory and nonperturbative embedding methods. These methodologies also take advantage of advances in numerical mathematics, computer science, and machine learning, where fast tensor algorithms such as tensor cross-interpolation techniques have been developed. We believe that by combining progress in these areas it will be possible to generate a new generation of predictive and systematically improvable algorithms for obtaining experimentally measurable properties of strongly correlated quantum materials, including angle-resolved spectroscopy, neutron spectroscopy, and resonant inelastic x-rays. Ultimately, we aim to unlock new insights into the behavior of quantum materials, which will have profound implications for future scientific and technological advancements.