Abstract

"Quantum Simulation of Strongly Correlated Phases

in Low-Dimensional Solid-State Systems"

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Understanding strongly correlated quantum phases remains a central challenge in condensed matter physics, as many exotic states, like superconductors, spin liquids, and topological effects, emerge from interactions beyond the reach of perturbative methods. This thesis explores solid-state quantum simulators as an alternative platform for investigating such phases, providing strong electronic correlations, high tunability, and direct access to spin Hamiltonians.

We first analyze moiré transition metal dichalcogenides heterostructures, where the effective moiré potential results in arrays of localized quantum dots with interactions controlled by the relative twist between monolayers and the dielectric environment. Using exact diagonalization and effective Hubbard modeling, we show that these systems host a rich set of correlated ground states, including generalized Wigner crystals and signatures of spin polarization driven by the Nagaoka mechanism. By projecting onto the single-occupied, low-energy spectrum, we obtain an effective spin model with ring exchange interaction, which, for moderate dielectric screening, favors a quantum spin liquid. A nematic valence bond solid is favored for stronger screening as a ground state.

In the second part, we focus on graphene nanostructures as building blocks for quantum spin chains. We design mixed-size nanographene chains that realize the Haldane phase with short correlation length by combining spin-1 triangulene units with spin-1/2 phenalenyls. Density matrix renormalization group simulations reveal a finite Haldane gap, localized edge states, nonlocal string order, and an entanglement spectrum with even degeneracies characteristic of symmetry-protected topological order. By tuning the number of spin-1/2 buffer sites, the correlation length can be continuously adjusted toward the Affleck–Kennedy–Lieb–Tasaki limit, offering a route to engineer short-range topological phases.

These results establish moiré heterostructures and nanographene chains as versatile solid-state quantum simulators of correlated and topological matter. They highlight the potential of nanoscale electronic systems to complement ultracold atom platforms, extending quantum simulation into regimes of strong interactions and experimentally accessible energy scales.