



PhD THESIS DEFENSE: Theoretical models for quantum simulators of novel materials and devices

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Over the past three decades, optically trapped ultra-cold atoms have served as a versatile platform for controlled exploration of numerous condensed matter phenomena. The successful fabrication of magic angle twisted bi-layer graphene (MATBG) has introduced a new paradigm for condensed matter physicists, while concurrently posing a novel challenge for the quantum simulation community. This thesis is devoted to addressing this problem, focusing mainly on the simulation of MATBG structures using ultra-cold atoms within its initial three chapters.

To overcome the issue of unit cell expansion resulting from rotation misalignment, in the first chapter we propose the concept of "twist-less twistronics" (twistronics, a term coined from twist and electronics). This innovative notion involves replacing the physical rotation of o

the layer with a light-modulated hopping amplitude between the layers. Enabled by the architecture of ultra-cold atoms, this approach yields quasi-flat bands, a pivotal ingredient for collective phenomena observed in Magic-Angle Twisted Bilayer Graphene (MATBG), achieved at significantly reduced unit cell size

The opening chapter also presents a suitable experimental set-up. Moreover, it provides a comprehensive theoretical framework, including tight-binding calculations and effective models derived from perturbative analysis. The second chapter delves into the topological properties of an analogous system, emphasizing the energy separation between the quasi-flat bands and the resulting spectrum. We demonstrate Quantum Anomalous Hall Effect across diverse parameter regimes, accompanied by an exhaustive phase diagram with respect to tunable parameter

In the third chapter, we extend our investigation to encompass onsite, density-density attractive interactions between lattice atoms. Employing the Hartree-Fock-Bogoliubov mean-field approximation, we consider all feasible interaction channels within/between layers and spins. This chapter aims to elucidate the relationship between band flattening, a fully controlled parameter in our system, and the emergence/size of a superconductive gap. Notably, we uncover a substantial enhancement in the critical (Kosterlitz-Thouless) temperature within the quasi-flat band regime at quarter filling, along with a comprehensive diagram illustrating superconducting order parameters corresponding to each interaction channel

The fourth chapter marks a departure from condensed matter simulations, delving into "special purpose quantum computing" within the context of quantum batteries. These devices, analogous to their classical counterparts, store and release energy on demand, a process inherently governed by the battery Hamiltonian. Our work establishes a novel framework for assessing quantum battery performance and setting fundamental bounds on two key attributes: power and capacity. We investigate the essential Hamiltonian terms of a for achieving quantum speed-up in battery charging

The last, fifth chapter describes the theoretical tools, that have been used to support the first experimental realisation of the Extended Bose Hubbard model with dipolar excitons. We discuss the parameters of interests and important observables, such as a structure factor and discuss both the exact diagonalization and mean-field methods, which were necessary to verify the observation of strongly correlated phases at half and unit filling

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