Model design and Computational solutions for quantum moiré systems

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Two-dimensional quantum moiré materials represent artificial superlattice structures in stacks of two or more 2d atomic crystals, including graphene, transition metal dichalcogenides, etc. The interplay between the quantum geometry of wavefunctions and strong long-range Coulomb interactions, is the key ingredients for understanding the complex phase diagram of correlated states such as metal, insulator and superconductors therein. In this talk, I will discuss our recent model design and computational developments to provide understanding of these correlation effects. Quantum Monte Carlo simulations to reveal the phase diagram of twisted bilayer graphene at charge neutrality (PRX 11, 011014(2021)) and the momentum space Monte Carlo method that can solve the long range Coulomb interactions in an unbiased manner (CPL 38, 077305 (2021)), as well as the density matrix renormalization group giving rise to quantum anomalous Hall state in the strong coupling regime (Nat Commun 12, 5480 (2021)), will be explained. Few open questions and future directions will be discussed.