Nagaoka ferromagnetism in moiré triangular superlattice complexes

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Moiré superlattice can be created by stacking two atomic layers of different materials [1, 2] and one can tune samples band filling factor through large ranges by varying gate voltage. Electronic properties can be controlled through readily accessible external parameters such as twist angle, making them good candidates for quantum simulators, realizing, for example, the triangular lattice Hubbard model [2,3]. Several phases related to interparticle interactions have been already observed, like Mott insulator states at one hole per superlattice unit cell or generalized Wigner crystal states at other partial fillings [3-5]. Within the most of the current research periodic systems are investigated, and approximate methods have to be used to determine the ground state properties, because full inclusion of correlations is not possible due to enormous size of the Hilbert space, even when its reduction due to translational symmetry is included. The advantage of studies of finite size systems is that correlations can be fully taken into account.

In this work, we consider different finite size fragments of moiré triangular lattice and analyze its magnetic properties when doped away from the half-filling. In such a case one can expect a transition from a nonmagnetic state to Nagaoka ferromagnetism [7]. This type of magnetism comes from correlations effects, or in other words, is due to constructive interference between different many-body configurations. Using exact diagonalization methods, we fully take into account correlations and determine conditions for appearance of Nagaoka ferromagnetism for one, two and three extra carriers above the half-filling. For different shapes of triangular lattice fragments, we determine critical value of interaction strength leading to a transition to spin polarized state. Finally, the size of Nagaoka polarons is analyzed.

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