Pinball-liquid phases in a triangular lattice

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A large variety of materials have a triangular lattice which can host a number of attractive strongly correlated and frustration-induced effects. Here, we focus on the exotic frustration-induced charge order, called a pinball-liquid (PL) phase [1], where lattice sites of a particular sublattice exhibit insulating properties (act as "pins" for charge carriers), while the rest of the lattice is conducting. To investigate the charge-ordering phenomenon we use the extended Hubbard model with repulsive onsite (U) and intersite (V) density-density interactions between electrons, and on the grand-canonical ensemble (arbitrary total charge density is allowed). We investigate a ground-state phase diagram of the triangular lattice with charge orders that are commensurate with a $\sqrt{3} \times \sqrt{3}$ supercell (3 sublattices). Following our work where the model is solved within the mean-field approximation (MFA) [2], we consider the possible pinball-liquid formation where the Mott localization is taken into account by means of the dynamical mean-field theory (DMFT) with the Lanczos procedure to solve Anderson impurity models [3]. The regions in the phase diagram can be outlined and identified by means of atomic-limit results [4], where the phases are named by integer occupation numbers of the three sublattices. The 200- and 220-regions are well-described within the MFA and hence, the DMFT predicts the previously found PL phase on a less-doped side of the 220-region [2]. Due to the particle-hole asymmetry, it is not found in the 200-region [2]. The 210-, 100-, and 221-regions are also found within the MFA, but without the Mott localization these regions are metallic only. The insulating and PL phases in these regions appear within the DMFT but the strong particle-hole asymmetry holds: only the 221-region and the hole-doped part of the 210-region host PL phases for U at least as high as $4D$ (D is a half-bandwidth of a noninteracting lattice). We have also found the intersite-interaction-driven PL phases in the 110- and 211-regions. These regions are not present in the MFA results that are generally incorrect for the $zV < 2U$ (z is a coordination number). The latter PL phases are rather symmetric with respect to the change of a sign of a chemical potential despite strong particle-hole asymmetry of the 110- and 211-regions themselves.

References:

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