Charge order within extended Hubbard model on frustrated lattices

A. Alekseev[1,*], A. Cichy[1,2], and K. J. Kapcia[1]

[1]Institute of Spintronics and Quantum Information, Faculty of Physics and Astronomy, Adam Mickiewicz University in Poznań, Uniwersytetu Poznańskiego 2, PL-61614 Poznań, Poland

[2]Institut für Physik, Johannes Gutenberg-Universität Mainz, Staudingerweg 9, D-55099 Mainz, Germany

[*]*aleksey.alekseev@amu.edu.pl*

A large variety of materials have lattices with geometrical frustration, such as triangular or kagome lattices. They are known to host various exotic and strongly correlated phenomena, among which superconductivity, exotic charge and magnetic orders, topological states, etc. It is especially relevant, since the geometrical frustration can significantly amplify strongly correlated effects. We investigate the extended Hubbard model (EHM) with repulsive onsite and intersite density-density interactions between electrons, and on the grand-canonical ensemble (arbitrary total charge density is allowed). Here we focus on commensurate charge-ordering phenomenon that is interesting on its own in various systems [1–5] and intriguingly interplays with superconducting phases. The thorough study of the model has been carried out using the mean-field approximation [1, 2], atomic-limit solution [3, 5], and dynamical mean-field theory [5, 6], which allowed to carefully interpret the results and track the factors affecting the phase diagram. It has been found that the ground-state phase diagrams show many interesting features and new phases when the total charge density is not fixed and all-encompassing range of chemical potentials is analyzed (electron and hole doping up till the fully occupied and unoccupied lattice). Most importantly, the frustration introduces very strong particle-hole asymmetry that can be seen in each phase and phase transition, including very asymmetric appearance of pinball-liquid and quasi-1D stripe phases in the triangular and kagome lattice, respectively. Moreover, due to a Van Hove singularity and a Dirac-delta level in noninteracting triangular and kagome systems, on one side of the phase diagrams the highly doped charge-ordered phase continuously transitions directly to a non-charge-ordered fully occupied insulator. Finally, our approach fully captures the phase-separation phenomenon that extensively appears in the found phase diagrams. We expect that the results are useful to describe highly tunable moiré superlattices that can be modeled by the triangular- and kagome-lattice EHMs, ultra-cold atomic gases on optical lattices that are described by the EHM, triangular-lattice organic conductors, and the kagome-lattice maretials that recently received a lot of researchers' attention.

References

[1] A. Alekseev, A. Cichy, K. J. Kapcia, Phys. Rev. B 112, 115155 (2025).

[2] A. Alekseev, K. J. Kapcia, Physica A 692, 131520 (2026).

[3] K. J. Kapcia, Nanomaterials 11 (2021) 1181.

[4] Z. Yeimer et al., Phys. Rev. B 114, 065104 (2026).

[5] A. Alekseev, A. Cichy, K. J. Kapcia, arXiv 2605.18575 (2026).

[6] A. Georges, et al., Rev. Mod. Phys. 68, 13 (1996).