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**Phase diagram in two-dimensional Hubbard model: variational cluster approximation**[1] ARMEN KOCHARIAN, California State University, KUN FANG, GAYANATH FERNANDO, University of Connecticut, ALEXANDER BALATSKY, Los Alamos National Laboratory, KALUM PALANDAGE, Trinity College — The Variational Cluster Approximation (VCA) is used to rigorously calculate the intrinsic phase diagram in bipartite two-dimensional (2d) Hubbard structures such as square and honeycomb lattice geometries with attraction and repulsion of electrons. The Mott-Hubbard gap, manifested as a smooth metal-insulator transition at finite $U > 0$ in both square and honeycomb lattices at half filling ($n = 1$), is in agreement with the generic 2d phase diagram. However, a density variation with the chemical potential displays their distinct structural differences away from half filling. Near $n = 1$ at equilibrium we found discontinuous transition in square lattices signaling a phase separation instability into an inhomogeneous state with hole rich (metallic) and hole poor ($n = 1$-insulating) regions. In contrast, a smooth density transition in honeycomb geometry describes a continuous evolution of homogenous (metallic) state. Incorporation of long-range input in VCA using U>0 and U<0 models displays antiferromagnetic and superconducting ground states respectively. The implication of VCA results to HTSCs, topological insulators as well as comparison to other studies is discussed. The VCA provides strong support for spontaneous phase separation instability found in our quantum cluster calculations.

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