Cluster dynamical mean-field theory study of Mott transition in the triangular lattice Hubbard model

HUNG DANG, Institute for Theoretical Solid State Physics, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany, XIAO YAN XU, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, KUANG-SHING CHEN, Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany, ZI YANG MENG, Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China, STEFAN WESSEL, Institute for Theoretical Solid State Physics, JARA-FIT and JARA-HPC, RWTH Aachen University, 52056 Aachen, Germany — In strongly correlated electron systems, geometric frustration can significantly affect the Mott metal-insulator transition. Using the dynamical cluster approximation, a cluster extension of the dynamical mean-field theory, we examine the evolution of the metal-insulator transition phase boundary as a function of temperature and interaction strength for the anisotropic triangular lattice Hubbard model as the degree of geometric frustration varies. We show that (i) the slope of this phase boundary changes systematically along with the frustration, and (ii) there exists a critical frustration at which this phase boundary is vertical. We discuss in details the connection between this critical degree of frustration and the suppression of the antiferromagnetic order due to frustration, which may be related to the emergence of exotic insulator phases as observed in several organic charge transfer salts.

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