Phase Diagram of a Half-filled Two-dimensional Ionic Hubbard Model

Chang-Qin Wu[a], Hui-Min Chen[a], Hui Zhao[b], and Hai-Qing Lin[c]

[a]Department of Physics, Fudan University, Shanghai 200433, China
[b]Department of Physics, Tongji University, Shanghai 200092, China
[c]Department of Physics, The Chinese University of Hong Kong, Shatin, Hong Kong, China

The quantum phase diagram of a half-filled two-dimensional ionic Hubbard model is investigated by the variational cluster approach (VCA).[1] For weak Coulomb repulsion U, the system is a band insulator (BI) with a band gap 2Δ induced by the alternative on-site energies $\pm\Delta$. For the strong-coupling limit $U \gg (\Delta, t)$, the Hamiltonian can be mapped onto an effective Heisenberg model where the ground state is a Mott-insulator (MI) with an anti-ferromagnetic long-range order. In this work, we present explicit evidence for the tendency toward a novel intermediate phase, the bond-located spin density wave (BSDW) phase characterized by a bond-located magnetization, in this model. To determine the possible phase between the BI and MI, we have used a variety of Weiss fields including the one for BSDW, which is found to be favored from an energy point of view. The phase diagram we obtained shows the width of BSDW region shrunk with increasing Δ. Whether there is a critical value Δ_c beyond which the BSDW vanishes is hard to be determined within the VCA. The bond-located spin density wave competes with the antiferromagnetism while the charge-density modulation exists all the way due to the staggered potential Δ.

[1]H.M. Chen, *et al.*, New J. of Phys. **12**, 093021 (2010) and reference therein.