Intermediate phase of the two-dimensional half-filled ionic Hubbard model

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Studies of the electron correlations induced metal-insulator transition are of considerable interest in condensed matter physics. The Hubbard model plays an important roll in understanding the effects of correlations for its ability to drive a transition to gapped MI, where the valence electrons are localized by the interaction U , with all sites singly occupied. On the contrary, there is a modulation of charge density in band insulators with one sub-band fully filled and the other empty. Recently some studies find a converse phenomenon that correlations produce delocalization effects on the electrons. The periodic external potential can lead to an insulating phase at $U = 0$, as a beginning in investigating the delocalization effect caused by U. As a result, much attention has been paid to the ionic Hubbard model, an extended version of the Hubbard model including a staggered on-site potential. Several types of insulators such as the BI and MI can be described within this simple model via tuning the strength of parameters.

We investigate the phase transitions in the half-filled ionic Hubbard model on a two-dimensional square lattice using the Lanczos exact diagonalization and variational cluster approximation. With increasing the Coulomb repulsion U, we find a phase transition from a band insulator (BI) to a Mott insulator (MI) with a possibly bond-ordered insulating (BOI) phase in between. Calculations of the charge gap and Drude weight indicate that the system is insulating for all parameters except at the phase boundary U_{C1} between the BI and BOI. The second phase transition to a MI at U_{C2} is accompanied by antiferromagnetic order and a finite charge gap. Our results are qualitatively and quantitatively consistent with those obtained by cluster dynamical mean field theory.