Abstract:
Motivated by the observation of inhomogeneous patterns in some high-Tc cuprate compounds, several variational Gutzwiller-projected wave-functions with built-in charge and bond order parameters are proposed for the extended t-J-V model on the square lattice at low doping. First, following a recent Gutzwiller-projected mean-field approach by one of us (Phys. Rev. B. bf 72, 060508(R) (2005)), we investigate, as a function of doping and Coulomb repulsion, the stability of the staggered flux phase with respect to small spontaneous modulations of squared unit cells ranging from 2× 2 to √32×√32.
It is found that a 4× 4 bond-order (BO) modulation appears spontaneously on top of the staggered flux pattern for hole doping around 1/8. A related wave-function is then constructed and optimized accurately and its properties studied extensively using an approximation-free variational Monte Carlo scheme. Finally, the competition of the BO-modulated staggered flux wave-function w.r.t. the d-wave RVB wave-function or the commensurate flux state is investigated. It is found that a short range Coulomb repulsion penalizes the d-wave superconductor and that a moderate Coulomb repulsion brings them very close in energy. Our results are discussed in connection to the STM observations in the under-doped regime of some cuprates.