GROUND STATE PROPERTIES OF ONE-DIMENSIONAL AND TWO-DIMENSIONAL HUBBARD MODEL FROM GUTZWILLER CONJUGATE GRADIENT MINIMIZATION THEORY

Zhuo Ye[(a)], Feng Zhang[(a)], Yong-Xin Yao[(a)], Cai-Zhuang Wang[(a)], Kai-Ming Ho[(a)]

(a) *Ames Laboratory of U.S. Department of Energy, and Department of Physics and Astronomy, Iowa State University, Ames, Iowa 50011, USA*

The Gutzwiller conjugate gradient minimization (GCGM) theory is an *ab initio* quantum many-body theory that we recently developed for computing the ground-state properties of infinite systems. GCGM is developed under the framework of the Gutzwiller wave function but does not use the commonly adopted Gutzwiller approximation (GA) to improve the accuracy. Instead, the theory uses an approximation that is based on the occupation probability of the on-site Fock states, rather than approximations that decouple the site-site correlations as used in the GA. The accuracy of the theory is demonstrated by evaluating the energy, the double occupancy and the spin correlation of the one-dimensional and two-dimensional Hubbard models at various electron densities. These observables are reproduced in reasonable agreement with benchmark data at a very small computational cost.