Variational Monte Carlo Study of Two-Dimensional Multi-Orbital Hubbard Model on Square Lattice

Y. Takenaka and N. Kawakami

Department of Physics, Kyoto University, Kyoto 606-8502, Japan

The Mott metal-insulator transition is an interesting and important issue in condensed matter physics. Especially, Mott transitions in multi-orbital systems have been investigated extensively. Prototypical examples are the orbital-selective Mott transitions in ruthenium alloys and the unconventional superconductivity in iron pnictides. In these systems, Hund's coupling as well as inter- and intra-orbital Coulomb interactions plays important roles. To understand the effects of orbital degeneracy, it is necessary to study these effects systematically.

In this study, we investigate a two-dimensional two-orbital Hubbard model on a square lattice at half filling. Applying the variational Monte Carlo (VMC) method, we address the Mott transitions in two-orbital systems. With this method, we can accurately estimate the ground-state properties. As a variational trial wave function, we consider Gutzwiller's on-site correlations and nearest-neighbor doublon-holon correlations because Mott transitions cannot be described correctly within Gutzwiller's wave function in finite dimensions. [1] We calculate the ground-state energy and obtain the phase diagram at zero temperature. The momentum distribution and the structure factors for the spin and charge density are also calculated. From these data, we discuss how Hund's coupling affects the Mott transitions in multi-orbital systems.

[1] H. Yokoyama and H. Shiba, J. Phys. Soc. Jpn. **59**, 3669 (1990)