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Spin-state transition and phase separation in multi-orbital Hubbard model SUMIO ISHIHARA, RYO SUZUKI, Department of Physics, Tohoku University, TSUTOMU WATANABE, Chiba Institute of Technology — Exotic phenomena in correlated electron systems are responsible for competition and cooperation between multi-electronic phases. In particular, in perovskite cobaltites, there is the spin-state degree of freedom, i.e., multiple spin states due to the different electron configurations in a single ion. The multiple spin states occur by changes in the carrier concentration, temperature and other parameters. In the lightly hole doped region between the low-spin band insulator (BI) and the high-spin (HS) ferromagnetic metallic (FM) states, several inhomogeneous features have been reported experimentally. We address the issues of the spin-state transition and the phase separation (PS) associated with this transition by analyzing the multi-orbital Hubbard model [1]. We examine the electronic structures in hole doped and undoped systems by the variational Monte-Carlo (VMC) method. We find that the electronic PS is realized between the nonmagnetic BI and the HS FM metal. We conclude that the different band widths play an essential role in the present electronic PS. [1] R. Suzuki, T. Watanabe, and S. Ishihara, Phys. Rev. B 80, 054410 (2009).

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