The effect of orbital fluctuations on the Mott transitions in the multiorbital Hubbard model

K. Inaba, A. Koga, S. Suga, and N. Kawakami

Department of Applied Physics, Osaka University, Suita, Osaka 565-0871.

Strongly correlated electron systems with some orbitals have attracted much interest. Among them, the orbital-selective Mott transition (OSMT) [1] has been one of the most active topics in this context. Typical materials are $Ca_{2-x}Sr_xRuO_4$ [2] and $La_{n+1}Ni_nO_{3n+1}$ [3], where the OSMT is suggested to be realized by the chemical substitution and the change in the temperature. One of the characteristic of the OSMT is the experimental observation of an unexpected localized spin S = 1/2 in the metallic system in $Ca_{2-x}Sr_xRuO_4$ for $x < 0.5$[2], which is difficult to obtain from the entirely itinerant description. These experimental findings have stimulated theoretical investigations of the Mott transitions in the multiorbital systems.

Motivated by this, we investigate the Mott transitions in two-orbital Hubbard systems by using the self-energy functional approach[4] and the dynamical mean-field calculations. We give a brief review of our recent studies [5]. In particular, we focus on the role of orbital fluctuations to discuss the stability of the intriguing metallic state which is induced by the OSMT. We also provide the phase diagrams at zero and finite temperatures (FIG. 1).

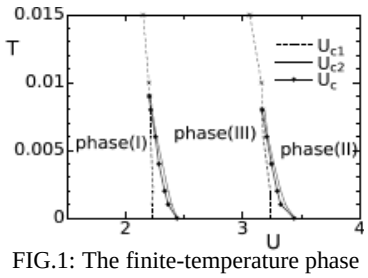

FIG.1: The finite-temperature phase diagram of the two-orbital Hubbard model with different bands [5]. In the phase (I) [(II)], both bands are in the metallic (insulating) state. The phase (III) is the intermediate state which is induced by the OSMT.

[1] V. I. Anisimov *et al*., Eur. Phys. J. B **25** (2002) 191.
[2] S. Nakatsuji and Y.Maeno, Phys. Rev. Lett. **90** (2003) 137202.
[3] Y. Kobayashi *et al*., J. Phys. Soc. Jpn. **65** (1996) 3978.
[4] M. Potthoff, Eur. Phys. J. B **32** (2003) 429; **36** (2003) 335.
[5] K. Inaba *et al*,, Phys. Rev. B **73** (2006) 155106; J. Phys. Soc. Jpn. **74** (2005) 2393; Phys. Rev. B **72** (2005) 085112; A. Koga *et al.*, Prog. Theor. Phys. Suppl. **160** (2005) 253.