(P2-29)

Incommensurate orbital state due to competition between itinerant and localized f-electron orbitals

Hiroaki Onishi and Takashi Hotta

Advanced Science Research Center, Japan Atomic Energy Agency, Tokai, Ibaraki 319-1195

To clarify a key role of orbital degree of freedom in f-electron systems, we have investigated the ground-state property of a one-dimensional three-orbital Hubbard model on the basis of a j-j coupling scheme, by exploiting a density-matrix renormalization group method [1]. Here, we consider a chain system along the z direction including one f electron per site, and investigate the cubic crystalline electric field (CEF) effect. The level splitting between Γ_7 and Γ_8 orbitals is controlled by a cubic CEF parameter B_4^0. Note that Γ_7 and Γ_8^a orbitals are localized, while Γ_8^b orbital is itinerant, due to the orbital shape, as shown in Fig. 1(a).

At B_4^0=0, three orbitals are degenerate, but we find that itinerant Γ_8^b orbital is favorably occupied to gain kinetic energy. When we increase B_4^0, electrons are forced to be accommodated in the lower Γ_7 orbital, and there occurs a characteristic change of the orbital state. In Fig. 1(b), we show the site dependence of the electron density in each orbital. With increasing B_4^0, it is observed that localized Γ_7 orbital is occupied at regular intervals. Such a site with Γ_7 orbital introduces a cut into the chain due to the absence of electron hopping. On the other hand, the sites in which itinerant Γ_8^b orbital is occupied get together and form clusters to gain kinetic energy. Thus, an incommensurate orbital state appears due to the competition between the itinerant nature of Γ_8^b orbital and the localized nature of Γ_7 orbital.

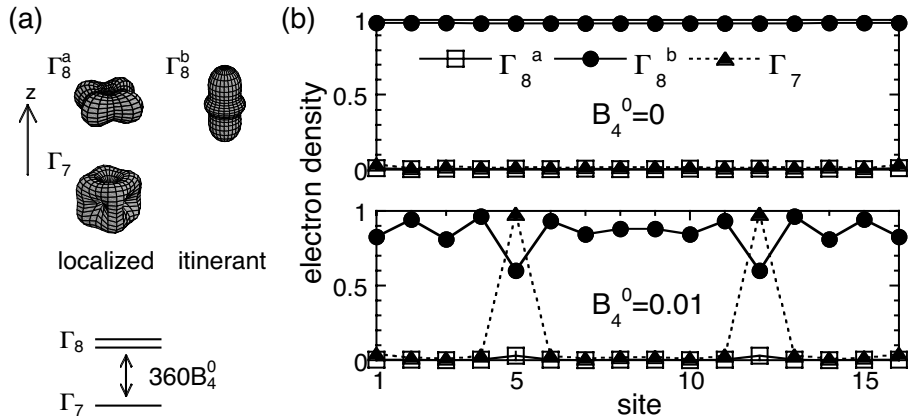

Figure 1: (a) Schematic views of Γ_7, Γ_8^a, and Γ_8^b orbitals. (b) Electron density in each orbital.

[1] H. Onishi and T. Hotta, cond-mat/0511276.