Numerical Study of Quarter-filled Extended Hubbard Chain coupled to Ising Spins

Yuichi Otsuka[1,2], Hitoshi Seo[1,2], and Yukitoshi Motome[3]
[1] *Condensed Matter Theory Laboratory, RIKEN, Japan*
[2] *CREST-JST, Japan*
[3] *Department of Applied Physics, University of Tokyo, Japan*
Email: otsukay@riken.jp

π-*d* systems, in which itinerant π-electrons are coupled to *d*-electrons, have recently attracted much interest in the field of the molecular conductors. For instance, extensive experimental efforts have been done for the one-dimensional (1D) conductor TPP[Fe(Pc)$(CN)_2]_2$, in which Fe ions provide localized *d* moments with large anisotropy. It has been argued that the charge order (CO) as well as the negative magnetoresistance phenomena observed in this compound is likely owing to the coupling between π-electrons and Fe moments [1]. To understand the intriguing properties in the π-*d* systems, we study finite-temperature properties of the 1D quarter-filled extended Hubbard model coupled to Ising spins via the ferromagnetic Hund's-rule coupling by Monte Carlo simulation. The antiferromagnetic (AF) superexchange (SE) interaction between the Ising spins is also included in the model, following the experimental observations. Our model shares some features with the ferromagnetic Kondo lattice-type models investigated in the context of the manganese oxides [2], while we pay special attention to the stability of the CO. We find that the Hund's-rule coupling, which tends to stabilize ferromagnetic metal through the double-exchange (DE) mechanism, competes with the intersite Coulomb repulsion, which causes the CO insulating behavior. Moreover, a competition between the DE interaction and the AF SE interaction results in complicated magnetic phase instabilities, which are also reflected to the charge degree of freedom. We will also discuss effects of magnetic field on finite-temperature properties, such as the susceptibilities and the CO correlation, and compare our results with the experiments.

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