Finite-temperature phase diagram of neutral-ionic transition in charge-transfer organic complexes

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Neutral-ionic (NI) transition accompanying charge transfer between different molecules has been studied for long time in organic complexes. For example, a typical compound TTF-CA shows temperature-driven first-order NI transition at T=80K under ambient pressure. Recent experiments on TTF-CA under high pressure have revealed a novel P-T phase diagram with three phases, which can be regarded as solid, liquid and gas phase in analogy [1]. Kishine *et al.* have studied this phase diagram by an effective spin-1 Ising model [2]. It is, however, left unsolved how quantum fluctuation of low-dimensional electron systems affects the NI transition.

In this talk, we study the P-T phase diagram of TTF-CA based on a 1D extended Hubbard model with Peierls-type electron-lattice interaction. One-dimensional quantum fluctuation of electrons along the stacking direction is treated by Stochastic Series Expansion (SSE), which is one of quantum Monte Carlo methods. We introduce the inter-chain Coulomb interaction within a mean-field level for reproducing finite-temperature phase transition. Neglecting thermal and quantum fluctuation of lattice degree of freedom, we self-consistently determine the lattice distortion and charge transfer by a mean-field theory. We show a schematic phase diagram determined by our calculation in Fig. 1. We also discuss relevance of our result to experiments on TTF-CA under pressure.

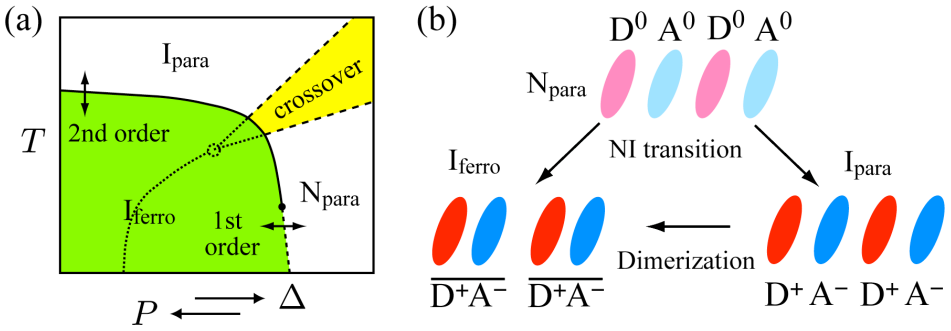

Fig.1 (a) A schematic phase diagram, and (b) the corresponding states for three phases. Here, D(A) denotes a donor(accepter) molecule.

[1] M. H. Lemée-Cailleau *et al.*, Phys. Rev. Lett. **79**, 1690 (1997); K. Kanoda, unpublished.
[2] J.-I. Kishine *et al.*, Phys. Rev. B **69**, 075115 (2004).