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혼합 상 망간산화물의 상 분리 및 유사 띠간격 연구

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Phase Separation and Pseudogap in Mixed Phase Manganites

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1. Introduction

The recent observation of colossal magnetoresistance (CMR) in doped manganites draws a great amount of interest in understanding their unusual magnetotransport properties.[1] One of the most notable feature of these material is that density of states in mixed-phase regimes reveal pseudogap characteristics, namely a prominent depletion of weight at the Fermi level.[2] Among the theories proposed for the pseudogap phenomenon are those based on the recently observed intrinsic inhomogeneities of models with nanometer size cluster toward phase separation where a ferromagnetic (FM) state is metallic and the other antiferromagnetic insulating. So far, however, there is no theoretical report on the transport properties in the phase separation region, even through it is essential to understand the intrinsic inhomogeneities of the mixed phase manganites.

2. Model and methods

The FM Kondo lattice model Hamiltonian including a strong Hund's coupling term as well as a hopping term is written by

$$H = -\sum_{\langle ij\rangle,\sigma}(t_{ij}c^{+}_{i\sigma}c_{j\sigma} + h.c.) - J_H\sum_{iab} S_i\ \sigma_{ab}c^{+}_{ia}c_{ib}$$

where σ_{ab} is the Pauli matrix for the conduction electron spins, S_i represents the localized spin of Mn electrons and $J_H > 0$ is the Hund's coupling, and the rest of the notation is standard. To study magnetotransport properties, a Monte Carlo algorithm for the localized spins and an exact diagonalization were used. Calculation were performed for the one-dimensional chain with L=48. The parameters used for the calculations were $J_H = 12t$, and $T = 0.02t$.

3. Monte Claro results

Figure 1 shows the density of states $N(w)$ vs $w-\mu$ for the various values of external magnetic fields near the mixed phase regime by adjusting $\mu = -10.4895$. In this regime, Monte Carlo calculation of temperature vs chemical potential revealed the presence of phase separation.[3] The most noticeable feature is the presence of the deep minimum at $w=\mu$, which clearly develops as external magnetic field is increased. Similar results have been obtained in other parts of parameter space, as long as the system is near phase separated regimes.[3]

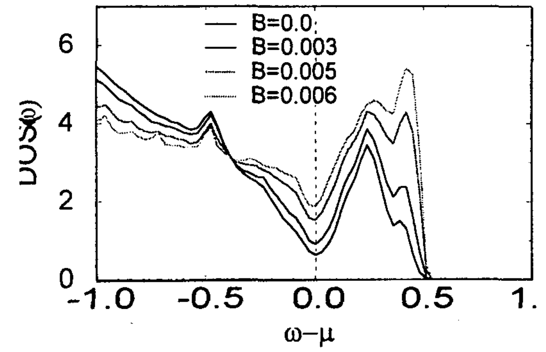

Fig. 1. $N(w)$ vs $w-\mu$

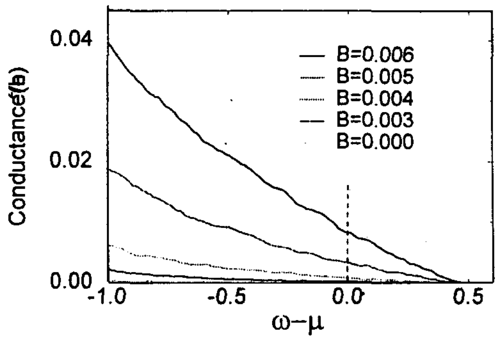

Fig. 2. Conductance vs $w-\mu$

To investigate the origin of the pseudogap, we calculated the conductances based on the Landauer formalism with ensemble averages over spin configurations generated by Monte Carlo simulations vs $w-\mu$, as shown in Fig. 2 at the region of interest. The absence of conductances at $w=\mu$ for the weak magnetic fields is compatible with the insulating characteristics of the reduction in $N(w)$. The conductances increase greatly in the presence of strong magnetic fields, indicating a metal-insulator transition, in a good agreement with the experiments.[2] This agreement adds to the notion that intrinsic inhomogeneities in mixed phase regime is important to understand the mechanism of the CMR effects.

4. Summary

We calculate the magnetic field dependence of the density of states and the conductances in the phase separation region using Monte Carlo simulations and Green function techniques. The conductances increase greatly in the presence of external magnetic fields, indicating a metal-insulator transition. We also find that the pseudogap results from a mixed phase of metallic and insulating states.

5. Reference

[1] Y. Tokura and N. Nagaosa, Science 288, 462 (2000).
[2] A. Moreo, S. Yunoki, and E. Dagotto, Phys Rev. Lett. 83, 2773 (1999).
[3] H. Yi and J. Yu, Phys. Rev. B 58, 11 123 (1998).