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Suppression of carrier spin polarization in diluted ferromagnetic semiconductors

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Abstract
We present a theoretical method for studying diluted magnetic semiconductors, extending the dynamical cluster approximation. The precursor effects of the localization and the direct exchange interaction between magnetic impurities can be considered in the method. We apply the method to the two-dimensional square lattice system with random localized spins. We show that the strong antiferromagnetic superexchange interaction between nearest-neighbour sites suppresses the polarization of the carrier spin.

1. Introduction

For more than two decades, diluted magnetic semiconductors (DMSs) have attracted attention because of their combined magnetic and semiconducting properties. Since the recent discovery of ferromagnetism in $In_{1-x}Mn_xAs$ and $Ga_{1-x}Mn_xAs$ [1], III–V-based DMSs have notably been of interest from the industrial viewpoint, because of their potentiality as new functional materials for realizing spin electronics (spintronics). For the purpose of designing DMSs with high Curie temperature T_C, a number of *ab initio* studies have been carried out. Recently, Akai carried out a detailed investigation of the ground state properties by using the Korringa–Kohn–Rostoker method combined with the coherent potential approximation, i.e., KKR-CPA theory [2], and Sato and Katayama-Yoshida have carried out a systematic characterization of the ground state magnetization along similar lines [3].

On the other hand, in addition to such *ab initio* calculations of specific materials, simple model calculations are also necessary to promote understanding of the general features [4–6]. The ferromagnetism in DMSs is generally considered to be induced by carriers, and

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much effort has been made to elucidate the origin of the carrier-induced ferromagnetism from various viewpoints. In spite of the apparent success of these theories, e.g., the mean-field theory, the Ruderman–Kittel–Kasuya–Yosida (RKKY) interaction and the double-exchange mechanism, there is still some shadow region concerning the effects of the disorder on the magnetism. Most current theories treat a doped magnetic impurity in the framework of the single-site approximation and neglect the nonlocal correlations due to the disorder. Thus, the precursor effects of the localization and the direct exchange interaction between neighbouring impurities are not satisfactorily taken into account. In this paper, we study the effects of the disorder on the itinerant carriers beyond the single-site approximation, using the dynamical cluster approximation (DCA) technique [7, 8]. The DCA was developed for ordered correlated systems such as the Hubbard model to add nonlocal corrections to the dynamical mean-field approximation. We extend the DCA to treat a disordered system with random magnetic impurities. We apply the method to the two-dimensional square lattice system with random localized impurity spins.

2. Formulation

We consider the following Hamiltonian, which is a good starting point for studying DMSs:

$$H = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} - \sum_{i} J^{C}_{i} \boldsymbol{s}_i \cdot \boldsymbol{S}_i + \sum_{ij} J^{S}_{ij} \boldsymbol{S}_i \cdot \boldsymbol{S}_j. \tag{1}$$

Our Hamiltonian has the two exchange interactions; one is that between the itinerant carrier and the localized spin J^{C}_{i} and the other is that between the neighbouring localized impurity spins J^{S}_{ij}. These are random variables: $J^{C}_{i} = J^{C}$ if the site i is occupied by a magnetic impurity and $J^{C}_{i} = 0$ otherwise. Similarly, $J^{S}_{ij} = J^{S}$ if both the sites i and j are occupied by magnetic impurities and $J^{S}_{ij} = 0$ otherwise. For a particular configuration of both substitution and spin orientation of the localized spin, the self-energy of the carrier differs according to the orientation of the carrier spin, and then the carrier spin becomes polarized. The polarization of the carrier spin induces polarization of the localized spins, in turn. Thus, the itinerant carrier and the localized spin should be treated self-consistently. In order to consider the effects of the disorder on the itinerant carriers, however, we simplify the problem, dividing (1) into the localized spin term and the itinerant carrier term:

$$H^{\mathrm{SPIN}} = \sum_{i} h^{\mathrm{eff}} S^{z}_{i} + \sum_{i,j} J^{S}_{ij} S^{z}_{i} \cdot S^{z}_{j}, \tag{2}$$

$$H^{\mathrm{CARR}} = \sum_{ij,\sigma} t_{ij} c^{\dagger}_{i,\sigma} c_{j,\sigma} - \sum_{i} J^{C}_{i} \boldsymbol{s}_i \cdot \boldsymbol{S}_i, \tag{3}$$

where h^{eff} is the field induced by the polarization of the carrier spin. For a certain substitutional configuration, the Boltzmann factor of the localized spin system, that is, the probability distribution of the configuration of the spin orientation, is determined by H^{SPIN}.

Following the DCA technique [7, 8], we divide the Brillouin zone into N_{c} equal cells (coarse-graining cells). The averaged cluster Green function is given by the coarse-grained Green function

$$\bar{G}(\boldsymbol{K}, \omega) \equiv \frac{N_{\mathrm{c}}}{N} \sum_{\tilde{\boldsymbol{k}}} \frac{1}{\omega - \epsilon_{\boldsymbol{K}+\tilde{\boldsymbol{k}}} - \Sigma^{\mathrm{DCA}}(\boldsymbol{K}, \omega)}, \tag{4}$$

specified by the cluster momentum $\boldsymbol{K}$. The $\tilde{\boldsymbol{k}}$ summation runs over the momenta of the cell about $\boldsymbol{K}$. Using the cluster-excluded propagator $\mathcal{G}(\boldsymbol{K}, \omega) = 1/[1/\bar{G}(\boldsymbol{K}, \omega) + \Sigma^{\mathrm{DCA}}(\boldsymbol{K}, \omega)]$, we calculate the cluster Green function for each configuration for both substitution and spin

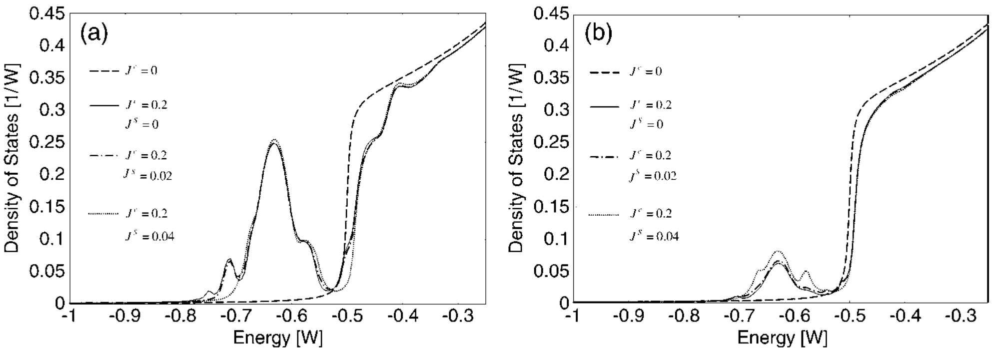

Figure 1. The density of states of (a) majority and (b) minority spin carriers for various J^S. $J^C = 0.4[W]$, $h^{\text{eff}} = 0.4[W]$ and the impurity concentration $n_i = 0.05$.

orientation of the localized spin, and then average over all possible configurations on a cluster of N_c sites. In this study, we consider multi-site scattering, including the spin flip processes within the single-site approximation [4, 6].

3. Calculated results

Because of the large calculation demanded in the DCA, as a preliminary study, we apply the method to a two-dimensional square lattice system with random spin moments $S = 5/2$. For J_{ij}^S, keeping in mind the superexchange interaction which is usually short range, we consider only the antiferromagnetic (AF) exchange interaction between nearest-neighbour sites and do not treat the other direct exchange interactions between the localized spins in this study. Indeed, the contribution to Σ^{DCA} from the impurity scattering involving the far impurity sites is small enough to be ignored. We take the bandwidth $W = 8t$ as the unit of energy. t is the nearest-neighbour transfer energy. The impurity concentration is $n_i = 0.05$. We show the spin polarized density of states (DOS) at $T = 0$ in figure 1. For $J^S = 0.04[W]$, the DOS of the majority spin carrier decreases and the DOS of the minority spin carrier increases, at low energy. Therefore, the polarization of the carrier spin is suppressed by the AF superexchange interaction. The results indicate that the neighbouring magnetic impurities not only couple antiferromagnetically to each other, but also reduce the carrier-induced ferromagnetic interaction. On the other hand, for $J^S = 0.02[W]$, the DOS hardly changes from that for $J^S = 0$. This is because the number of configurations where the localized spins are coupled by the weak J^S is small. While we consider the two-dimensional system here, the two-dimensional nature of the system does not play an important role in Σ^{DCA} because the interaction between carriers is not considered and the localized spin is treated as a classical spin in our formulation. Thus, the suppression of the polarization of the carrier spin due to the AF superexchange interaction still holds for the three-dimensional DMSs.

4. Summary

We have presented a theory for use in studying the effects of disorder on the itinerant carriers in DMSs, extending the DCA to treat a disordered system with random magnetic impurities. We applied the method to the two-dimensional square lattice system with random spin moments. We found that the strong AF superexchange interaction suppresses the polarization of the carrier spin.

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References

[1] Ohno H 1998 *Science* **281** 951
Ohno H 2001 *Science* **291** 840
[2] Akai H 1998 *Phys. Rev. Lett.* **81** 3002
[3] Sato K and Katayama-Yoshida H 2000 *Japan. J. Appl. Phys.* **39** L555
[4] Takahashi M and Kubo K 2002 *Phys. Rev.* B **66** 153202
[5] Yagi M and Kayanuma Y 2002 *J. Phys. Soc. Japan* **71** 2010
[6] Bouzerar G, Kudrnovský J and Bruno P 2003 *Phys. Rev.* B **68** 205311
[7] Hettler M H, Tahvildar-Zadeh A N and Jarrell M 1998 *Phys. Rev.* B **58** R7475
[8] Jarrell M and Krishnamurthy H R 2001 *Phys. Rev.* B **63** 125102