A New Mean Field Theory for Ising Spin-Fermion Model: Application to Diluted Magnetic Semiconductors

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Abstract

We have investigated the ferromagnetic transition of an Ising spins-fermions model, where Ising spins are located randomly and tight-binding fermions interact with the Ising spins via the exchange interaction. We extended the inhomogeneous mean field theory to include the local dynamics of localized spins and applied to this model. We have found that the ferromagnetic moment is not saturated because of localization of fermions due to the randomness.

Key words: diluted magnetic semiconductors; mean field theory; ferromagnetism

Diluted magnetic semiconductors (DMSs) have long been of great interest. Especially, III-V based materials show rather high ferromagnetic transition temperature [1–3]. About this ferromagnetic transition several theories appeared recently [4–6].

Among these theories, we use following Ising spins-fermions model [6] as a model of DMS's;

$$\mathcal{H} = -t\sum_{\langle ij\rangle\sigma}\left(C^{\dagger}_{i\sigma}C_{j\sigma} + \text{h.c.}\right) + J\sum_{j,\sigma}^{imp.} S_j\sigma C^{\dagger}_{j\sigma}C_{j\sigma}, \quad (1)$$

where S_j is an Ising spin on a impurity atom, $\sum_j^{imp.}$ is a summation over the impurity atoms and J is an exchange interaction constant between localized spins and carriers.

We have solved this Hamiltonian in real space and incorporated spatial distribution of the magnetic order and dynamics of the localized spins. We consider i-th impurity site, and take thermal average of spins on the other sites j as,

$$\langle S_j\rangle = M_j \qquad (j \neq i). \quad (2)$$

However, the spin on the i-th site may become up or down. Then the local mean field (MF) Hamiltonian for the case when the spin on the i-th site is $S(= \pm 1)$ is written as,

$$\mathcal{H}_{\text{LMF}}\ (i,S) = -t\sum_{\langle ij\rangle\sigma}\left(C^{\dagger}_{i\sigma}C_{j\sigma} + \text{h.c.}\right) + J\sum_{j\neq i} M_j\sigma C^{\dagger}_{j\sigma}C_{j\sigma} + JS\sum_{\sigma}\sigma C^{\dagger}_{i\sigma}C_{i\sigma}. \quad (3)$$

We write the energy eigenvalues and eigenvectors of this Hamiltonian as,

$$\mathcal{H}_{\text{LMF}}\,(i,S)\,|\psi_{n\sigma}\,(i,S)\rangle = E_{n\sigma}\,(i,S)\,|\psi_{n\sigma}\,(i,S)\rangle\,, \quad (4)$$

$$|\psi_{n\sigma}\,(i,S)\rangle = \sum_j \psi_{n\sigma j}\,(i,S)\,C^{\dagger}_{j\sigma}\,|0\rangle\,. \quad (5)$$

Solving Eq.(4), we get the local eigenvalues $E_{n\sigma}\,(i,S)$ and eigenfunctions $\psi_{n\sigma i}\,(i,S)$. Then we can calculate the local partition function for the i-th site with S spin,

$$\Xi\,(i,S) = \prod_{n\sigma}\left\{1 + \exp\left[-\beta\left(E_{n\sigma}\,(i,S) - \mu\right)\right]\right\}, \quad (6)$$

where $\beta = 1/k_BT$ and μ is a chemical potential. Then thermal average of the localized spin on the i-th site is given by,

$$M_i = \frac{\Xi\,(i,\uparrow) - \Xi\,(i,\downarrow)}{\Xi\,(i,\uparrow) + \Xi\,(i,\downarrow)}. \quad (7)$$

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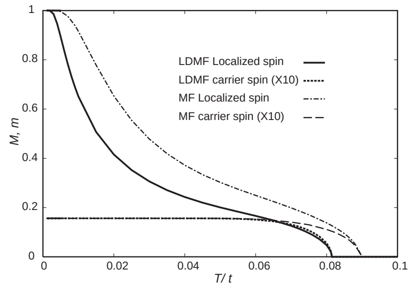

Fig. 1. Temperature dependences of ferromagnetic localized and carrier moments from LDMF and MF calculations.

For each impurity site, we solve eigenvalue equations and calculate the thermal average of the localized moment. The chemical potential μ is determined using each local partition functions as,

$$N_e = \sum_{i\sigma} \frac{\sum_S n_\sigma (i, S)\, \Xi (i, S)}{\sum_S \Xi (i, S)}. \qquad (8)$$

Here N_e is a total number of carriers and $n_\sigma (i, S)$ is the average number of the carrier with σ spin on the i-th site for localized spin S, which is given as,

$$n_{i\sigma} (i, S) = \sum_n |\psi_{n\sigma i} (i, S)|^2 f (E_{n\sigma} (i, S) - \mu), \qquad (9)$$

where f is the Fermi distribution function.

We start from an initial configuration of the averaged localized spins, then solve these equations self-consistently. We call this approximation as locally dynamical MF (LDMF).

First we have considered a case where localized spins are located every site in a two dimensional square lattice. We have taken 8×8 square lattice and set $J/t = 1$. In Fig.1, we show temperature dependence of the ferromagnetic moment for $N_e = 1$ from LDMF approximation and also a result from MF approximation. The result of LDMF shows lower transition temperature because of the local fluctuation of the localized spins. In Fig.2, we show the stable state for $N_e = 26$ and $T/t = 0.01$. In Ref.[6], around this carrier filling, the ferromagnetic state becomes unstable in their CPA approach, which cannot treat the spatial modulation of the magnetization. This state looks like the stripe state of the strongly correlated electron systems [7].

Second we have considered a three dimensional cubic lattice with a few randomly located magnetic impurity sites. In Fig. 3, we show typical distribution of localized moment for 10 impurity spins and $N_e = 6$, where the system size is $8 \times 8 \times 8$. In this configuration, only less than half of the spins are ferromagnetically ordered. Also carrier spins are concentrated around ferromagnetic moments as shown in Fig. 4. Such incomplete ferromagnetism may come from the randomness of the localized spins.

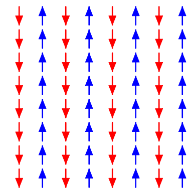

Fig. 2. Distribution of localized moments for $J/t = 1$, $N_e = 26$ and $T/t = 0.01$. The magnitude of the localized moment is $|M_i| = 0.98$.

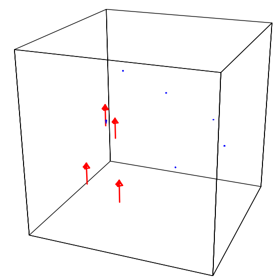

Fig. 3. Distribution of localized moments for $J/t = 7$, $N_e = 6$ and $T/t = 0.01$.

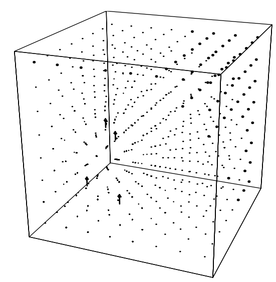

Fig. 4. Distribution of spins of carriers for $J/t = 7$, $N_e = 6$ and $T/t = 0.01$.

In summary, we have developed locally dynamical mean field approximation and we have obtained the spatial distribution of the localized ferromagnetic moments in DMS. Comparison with the experiment is a future problem.

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