

STABILITY OF METALLIC FERROMAGNETISM: CORRELATED HOPPING OF ELECTRONS IN Mn_4N *

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We study the ferromagnetic phase stability in Hubbard model in Mn_4N solid solution. It is believed that strong ferromagnetic orders in some solids are generated by subtle interplay between quantum many-body effects and spin-independent Coulomb interactions between electrons. Here we describe our numerical approach to ferromagnetism in the Hubbard model, which is a standard idealized model for strongly interacting electrons in a solid. We consider the correlated hopping of electrons in two-dimensional Hubbard model, to investigate the stability of ferromagnetism in Mn_4N solid solution with a Monte Carlo simulation. The ferromagnetic transition in double-correlated hopping model is studied by the Monte Carlo method and we determined the critical temperature involved in this process.

1. INTRODUCTION

The theoretical model of manganite materials, based on double-exchange (DE) interaction, was given in 1951 by Zener and has long been regarded as satisfactory. The ferromagnetic stability in Mn_4N solid solution is studied by the interference between the localized magnetic moment of Mn ions and the itinerant picture of the electrons. The correlated interaction of the band electrons was given by a Hubbard Hamiltonian like [1]:

$$H = - \sum_{i,j,\sigma} t_{ij} \hat{c}_i^\dagger \hat{c}_j + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \quad (1)$$

The pure Mn has an *FCC* type lattice and an antiferromagnetic alignment of the Mn spins. The antiferromagnetic behavior of the *FCC* Mn is given by the correlated interactions of the electrons [6]. By the existence of interstitials N atoms it is created a bridge between the electronic hoppings (the N been magnetic inert). This is a DE (Zener) interaction where are involving the two

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types of atoms Mn (with a magnetic influence) and N (without a magnetic behavior). The Hubbard interaction U represents the Coulomb repulsion of electrons in the same orbital at a given lattice site. It is given by the matrix elements [2]:

$$U = \langle ii | V(\vec{r} - \vec{r}') | ii \rangle \quad (2)$$

of the Coulomb potential, and is typically on the order of a few eV [3]. The t_{ij} matrix determines the inter-site hopping of itinerant electrons and is generally smaller than U , but may not be negligible small [4]. The operators $\hat{c}_{i\sigma}^+$, $\hat{c}_{i\sigma}$ indicate the creation and the annihilation operators of an electron and, $\hat{n}_{i\uparrow}$, $\hat{n}_{i\downarrow}$ are the number of particle operators (with spin up and down). This is the classical Hubbard Hamiltonian which is a good instrument of the band ferromagnetism theory in the pure magnetic systems.

2. PHYSICS MODELS

To explain the magneto-conductive properties of manganites, in which the manganese is present in at least two different valence states (Mn^{3+} and Mn^{4+}), Zener proposed the mechanism of double exchange (DE). The Mn 3d levels are split into two subsets: t_{2g} (threefold degenerate) and e_g (twofold degenerate). The t_{2g} electrons, lower in energy, are more localized. The outermost e_g electrons are more delocalized, capable of hopping from site to site provided that the t_{2g} spins on adjacent manganese atoms are parallel. According to the Jahn–Teller effect, as soon as an electron hops into an empty e_g orbital, a distortion of the cage of O atoms lowers the symmetry and further splits e_g and t_{2g} levels. The electron is now more tightly bound, forming a so-called lattice polaron. According to DE, the alignment of adjacent localized t_{2g} spin on manganese atoms rules the dynamics of itinerant e_g carriers, which hop from one atom to the next to yield electrical conductivity [12]. If adjacent t_{2g} spins are parallel (the ferromagnetic state), conduction is favored; if they are randomly aligned (the paramagnetic high-temperature state), conductivity drops dramatically. We proposed a Double – Correlated Hopping (DCH) model in Mn_4N , where the interstitials N can play the role of a bridge–hopping of the itinerant electrons. The hopping of the electrons is helped by the existence of N and thus the adjacent Mn spins are correlated with N participation. The double-correlated hopping model is described by the following Hamiltonian:

$$H = - \sum_{i,j,\sigma} t_{ij} \hat{c}^+(i) \cdot \hat{c}(j) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} - J_H \sum_{i,\sigma} \vec{s}_\sigma(i) \vec{S}_\sigma(i) \quad (3)$$

where u is the Coulomb interaction, t_{ij} is the hopping integral, $c^+(i) = (c_{\uparrow}^+(i), c_{\downarrow}^+(i))$ is the creation operators and $c(i) = (c_{\uparrow}(i), c_{\downarrow}(i))$ is the annihilation operators. Also, $\vec{s}_{\sigma}(i) = \frac{1}{2} c^+(i) \cdot \vec{\sigma} \cdot c(i)$ is the spin density operator of the conduction – electrons and $\vec{\sigma}$ is the vector of Pauli matrices, $\vec{S}_{\sigma}(i)$ is the localized spin and J_H is the ferromagnetic Hund coupling ($0 < J_H < \infty$).

3. MONTE CARLO ALGORITHM

The Monte Carlo (MC) simulations are done in N^3 cubic lattices with periodic boundary conditions. Although the localized spins are considered classical, the kinetic energy of the conduction electrons is calculating by diagonalizing the DE Hamiltonian [11]. The standard Metropolis algorithm was used in the MC simulations. The spin random reorientation on the site i , will induce the energy change ΔE . If the quantity $\exp(-\Delta E/KT)$ is smaller than a random number between 0 and 1, the change is allowed, otherwise it is rejected [10]. The average of the magnetization, m , are [13]:

$$m = \frac{1}{N^3} \left\langle \left| \sum_i \vec{S}_i \right| \right\rangle \quad (4)$$

where $\langle \rangle$ denotes statistical average. Due to the finite size of the unit cells used in the simulations, m is different from zero at any temperature, but we define the critical temperature T_C , as the point where the second derivative of m , change the sign.

4. RESULTS

In Fig. 1 we plot the magnetization versus temperature for the FCC lattice of Mn_4N , with interstitials N .

Thus we can approximate the critical temperature T_c , for different Hund's rule coupling and we can provide the influence of this parameter by the stability of ferromagnetism.

In Fig. 2 we show the critical temperature versus J_H (Hund coupling). This figure describes the phase diagram and provides a stabilization of ferromagnetic state for $J_H > 2$.

It is evident that the increase of the Hund's coupling leads of the stability of the magnetic ordered states (ferromagnetic alignments of magnetic spins).

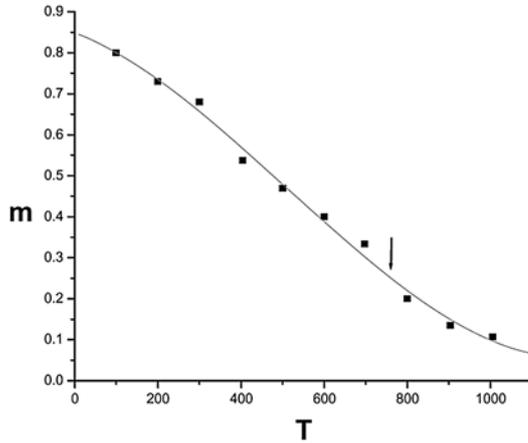


Fig. 1 – Magnetization versus T , at $N = 20$, with $n = 1.25$ and $J_H = 6$, $U = 6$.

In Fig. 3 we plot the dependence of critical temperature *versus* the electron densities n .

The ferromagnetic phase is found in a broad range of fillings. The maximum of the critical temperature is observed around $n = 1.25$. Closed $n = 2$ (half filling) is observed the antiferromagnetic phase, because the anti-ferromagnetic Heisenberg exchange suppresses the ferromagnetic order. We can say that the N atom play the role of an electronic bridge that produce a ferromagnetic adjacent alignment of the Mn atoms. This is a hybrid exchange model, between the Hubbard model and the Double-Exchange (DE) model. The existence of ferromagnetic state is conditioned by the range of itinerant electronic density. Around $n = 1.25$, the ferromagnetic state is characterized by a critical temperature around 800 K, very closed by the experimental results reports by I. Pop [14, 15].

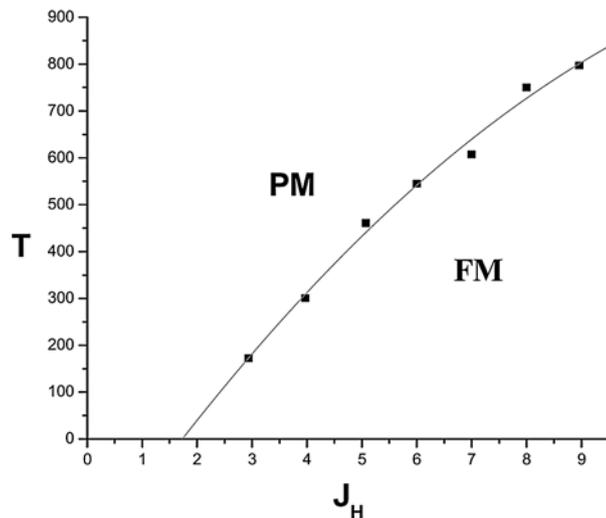
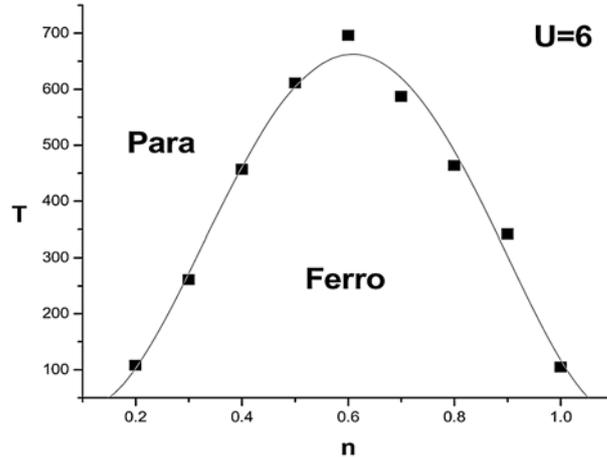


Fig. 2 – Curie temperature versus Hund's rule coupling, for $n = 1.25$, $U = 6$.

Fig. 3 – Magnetic T - n phase diagram for $U = 6$ and $J_H = 5$.



5. CONCLUSIONS

We used a Monte Carlo Algorithm to describe the ferromagnetic state in Mn_4N solid solution. The physics model is a hybrid model between the Hubbard model and Zener model. In our double – correlated hopping model the N atom is a bridge atom, magnetically inert that play the role of an intermediate hopping position. Thus, we can find the phase diagram with two type parameter: Hund's coupling and itinerant electronic density. Also we can approximate the critical temperature of Mn_4N in a metallic state ($n = 1.25$) with an intermediate electronic interaction ($J_H = 6$ and $U = 6$).

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