ELECTRONIC CORRELATION APPROACH IN ITINERANT FERROMAGNETISM*

EUGEN BIRSAN[1], COSMIN CANDIN[2]

[1] Physics Department, University "Lucian Blaga", Dr I. Ratiu str., No.5-7, 550024, Sibiu, Romania, beneugen10@yahoo.com

[2] Faculty of Engineering, University "Lucian Blaga" of Sibiu, Romania

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The microscopic origin of itinerant ferromagnetism were gained from investigations of electronic lattice models within Dynamical Mean-Field Theory (DMFT). We study the existence of metallic ferromagnetism in the one-band Hubbard model, which help to clarify the origin of band-ferromagnetism as a electronic correlation phenomenon. DMFT permits to investigate the stability of metallic ferromagnetism in intermediate values of the Coulomb onsite interaction U, and density n in 2D Monte Carlo (MC) simulation. We study the *T versus n* phase diagram of the Hubbard model as obtained within DMFT. In the present paper all DMFT results were obtained by Monte Carlo technique. We find the magnetic phase diagram in *T-n* dimensions and we conclude that the ferromagnetic state is extended in a large range of electronic density.

1. INTRODUCTION

Since the critical temperature of ferromagnetic metals like Fe, Co, Ni is of the order of electrostatic energies in solids, *i.e.* is much higher than the interaction energy of the electron spins, itinerant ferromagnetism is expected to be the result of the interplay between the ordinary spin-independent Coulomb interaction and the kinetic energy of the electrons, in combination with Pauli principle. The theory of itinerant ferromagnetism was investigated in two different modes: one using the many-body techniques and the other employing density functional theory (DFT) [1]. DFT are highly successful techniques for the calculation of electronic structure of the real materials. The one-band Hubbard model [13] was introduced to gain insight into the origin of metallic ferromagnetism. However even for this simplest possible microscopic model answers are not easily obtained since in general metallic ferromagnetism occurs at intermediate couplings and off half filling.

The dynamical mean-field theory (DMFT) is well-suited for the investigation of correlated electronic systems with strong local interactions [14]. It

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becomes exact for $d = \infty$, *i.e.*, for lattices with coordination number $Z = \infty$. Already in $d = 3$, the coordination number of regular lattices such as the FCC lattice, is quite large ($Z_{FCC} = 12$) and this natural to consider the limit $Z \to \infty$. To obtain a meaningful model in this limit one has to scale the NN hoping amplitude in the kinetic energy as $t = t^* / \sqrt{Z}$ (we set $t^* = 1$ for fix energy scale). Then one obtains a purely local theory where the self-energy $\Sigma_k(\omega)$ becomes $\vec{k}$ independent and where the propagator [12]:

$$G\left(\vec{k}, \omega\right) = G^{\circ}\left(\vec{k}, \omega - \Sigma(\omega)\right) \tag{1}$$

may be represented by the non-interacting propagator at a shifted frequency. In DMFT the information about the lattice or the dispersion of the system under investigation enters only through the density of states (DOS) $N^{\circ}(E)$ of the non-interacting particles, unless there is long-range order with broken translational symmetry of the lattice as the case of antiferromagnetism.

2. THE HUBBARD MODEL

The one-band Hubbard model characterized by the Hamiltonian:

$$H = -\sum_{i,j,\sigma} t_{ij} c_{i\sigma}^{+} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} \tag{2}$$

is the simplest lattice model for correlated electrons, and was proposed to understand metallic ferromagnetism in 3d transition metals [13].

Here, t_{ij} is a general hopping matrix element between sites i and j. The kinetic energy is usually restricted to nearest-neighbour (NN) hopping. Sometimes in addition to NN hopping t, longer-range hopping, in particular next-nearest-neighbour (NNN) hopping, t' is considered [8]. The Hubbard model is characterized by a local interaction term; therefore the kinetic energy of the electrons and the structure of the lattice are very important for the stability of metallic ferromagnetism. The NNN further-range hopping ($t' \neq 0$) is favourable to stabilization of itinerant ferromagnetism. If we consider a symmetric DOS, the fully polarized state is obtained by inverting the spin of the down electrons, witch due to the Pauli principle have to occupy higher energy states. The energy difference between the fully polarized state and the unpolarized state [7]:

$$\Delta E = \left[\int_{-W_1}^{u_{\uparrow}} - 2 \int_{-W_1}^{u} \right] N^{\circ}(E) E dE \tag{3}$$

must become negative for the ferromagnetic state to be stable. To obtain that $\Delta E < 0$, for $U > 0$, is one of the most difficult problems of electronic correlation theory.

3. FCC LATTICE

The itinerant ferromagnetism is an intermediate-coupling problem which doesn't obey an analytic solution. Investigations of the stability of metallic ferromagnetism on FCC lattices within DMFT in combination with QMC techniques (Quantum Monte Carlo) [14] provide a good correlation with experimental dates. To find a ferromagnetic instability one calculates the temperature dependence of the uniform static susceptibility χ from the corresponding two-particle correlation function. At an interaction strength of $U = 6$ the ferromagnetic response is strongest around $n = 0, 62$, where n is the electronic density. The susceptibility obeys a Curie-Weiss form, and thus the critical temperature can be extrapolated from the zero of $1/\chi$ [3]. The data points of magnetization are consistent with Brillouin function, and with the non-integer magneton number, in agreement with experiments in 3d transition metals [6].

Magnetization $m = m(T)$ is calculated by DMFT for the one – band Hubbard model with a density of states (DOS) given by [11]:

$$N_{FCC}(E) = \frac{e^{-\left(1+\sqrt{2}E\right)/2}}{\sqrt{\pi\left(1+\sqrt{2}E\right)}} \tag{4}$$

4. SIMULATION'S RESULTS

In Fig. 1 we plot the results graphic of the magnetizations versus temperature that presents Brillouin dependence. The critical temperature is finding around 650 K:

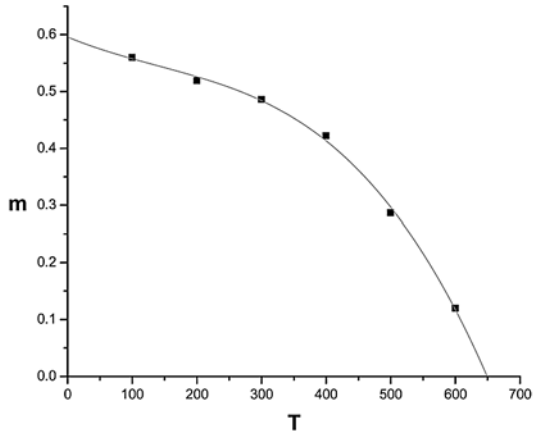


Fig. 1 – Magnetization *versus* *T*. Coulomb interaction is $U = 6$ and the electronic density is $n = 0, 62$.

It is also shown the susceptibility χ *versus* T in Fig. 2. We see that the susceptibility obeys a Curie-Weiss law:

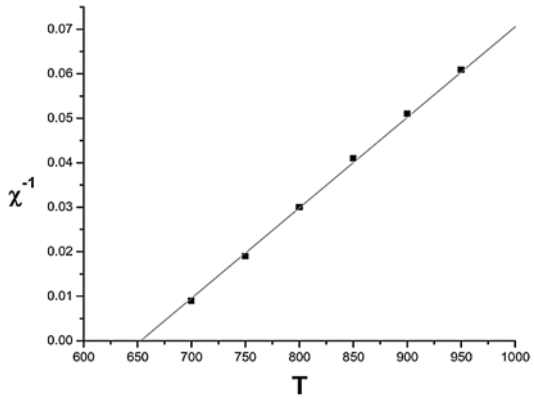
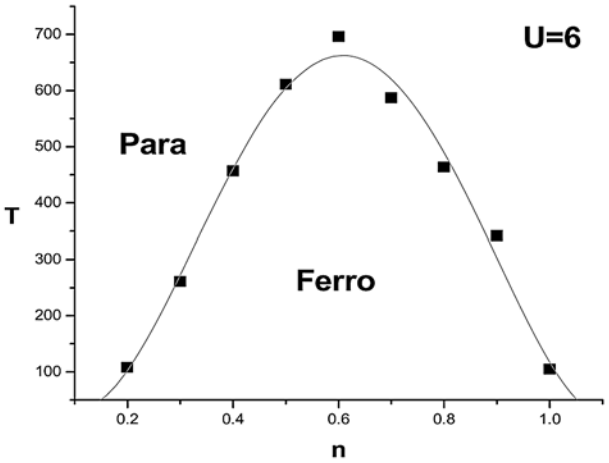


Fig. 2 – Magnetic susceptibility *versus* T.

The temperature $T_C = 650$ K is the value of the extrapolation $1/\chi \to 0$. Collecting the values of $T_C(U, n)$ obtained by $1/\chi(T_C, U, n) = 0$, the boundaries between the ferromagnetic and paramagnetic domains are determined. Thus one can provide the *T versus n* phase diagram for different values of U. For $t' = 0$, no instability is found at temperatures corresponding to QMC access. Already a small contribution of t' – hopping (which is present in any real system) is enough to stabilize a large region of metallic ferromagnetism in addition to an antiferromagnetic phase (which is absent in $d = \infty$), close to half filling.

Fig. 3 – *T versus n* phase diagram obtained within DMFT for an FCC lattice with NN hopping $t' = t/2$, in Hubbard model.



It is evident that in one-band Hubbard model, metallic ferromagnetism is found to exist in a large region of the U versus n phase diagram. The Coulomb interaction is a very important parameter to study the stabilization of ferro-

magnetism in metallic systems and the polarized state is more extended than the values of U, increase. It is evident that the present mechanism is perfectible with consideration of the band – degenerated Hubbard model. In real systems this approach is a good work to explain the existence of the ferromagnetic domain of the U *versus* n phase diagram. For example in Mn, where the FCC lattice leads to a strongly asymmetric DOS, this method is very powerful to provide the ferromagnetic state in a Hubbard model band degeneracy. Metallic ferromagnetism at weak coupling, usually known as Stoner ferromagnetism, has ruled out a long time ago based on the argument that the renormalization of the interaction strength brought about by T – matrix effects would never allow the Stoner criterion to be satisfied when the density of states at the Fermi level $\rho(E_F)$ is non singular. Physically, the largest possible effective interaction is equal to the kinetic – energy costs for making the two-particle wave function vanish when the two particles are at the same site. The energy scales like the bandwidth $\rho(E_F)^{-1}$ so that the Stoner criterion $1-U\rho(E_F)=0$ cannot be fulfilled. If there is Stoner – ferromagnetism in weak to intermediate coupling one needs at a singular density of states (DOS). An example of a model with singular DOS at the Fermi energy as well as band asymmetry is the two – dimensional (2D) Hubbard model with both nearest neighbor (NN) t and next nearest neighbor t' hopping. At weak to moderate values of the on-site Coulomb repulsion U, for small t'/t and close to half-filling the 2D Hubbard model $(t-t')$ shows an antiferromagnetic instability. Thus the t' parameter of hopping is very important for the stabilization of the magnetic state.

5. CONCLUSIONS

We study in DMFT technique the stability of ferromagnetism in FCC metallic lattice (like Mn, for example). We determined the magnetization and critical temperature in this lattice in the Hubbard model with intermediate Coulomb interaction (U). We also find the susceptibility, that obeys a Curie-Weiss law and the phase diagram of ferromagnetic transition in (T, n) coordinates and we determined the maximal transition temperature.

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