Magnetic properties of correlated electrons

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Abstract

We analyze a system composed of itinerant electrons and localized spins with on-site interactions representing the Hund’s first rule. Properties of the system are studied rigorously on the infinite square lattice but the configurational space is restricted to the lowest-period phases only. Using exact expressions for the ground state energy an evolution of the phase diagram with an external magnetic field is determined. For a wide range of electron densities metamagnetic phase transitions are detected. It is shown that jumps of magnetization of the electrons at the metamagnetic transitions are much smaller than changes of magnetization of the localized spins.

I. INTRODUCTION

In this paper we consider a model of localized spins and moving electrons on the square lattice. The spins do not interact between themselves directly, but only by means of the electrons. The interaction is local (on-site), however, since the electrons move, it spreads out over the whole system. According to the Hund’s first rule we assume the coupling between the localized spins and the spins of moving electrons to be ferromagnetic and, for simplicity, we choose the Ising-type anisotropy of the interaction.

The model can be viewed as a simplified version of the Falicov-Kimball model with the Ising on-site interaction we studied in our precedent papers. Indeed, if in the later model we impose exactly one localized \( f \)-electron per site then the only relevant terms that left are those given in the first line of the Hamiltonian (1). However, now we include also Zeeman type terms describing action of the magnetic field on both the localized spins and the electrons.

A type of magnetic order results from a competition between all the terms of the Hamiltonian. The Hund’s term and the magnetic field terms tend to align all the spins ferromagnetically. On the other hand, the kinetic energy term gives a favour of the antiferromagnetic order at half filling and close to that point.

The model Hamiltonian has the following form.

\[
H = t \sum_{\langle i,j \rangle} \sum_{\sigma = \uparrow, \downarrow} d_{i,\sigma}^\dagger d_{j,\sigma} - \mu \sum_i (n_{i,\uparrow}^d + n_{i,\downarrow}^d) - J \sum_i (n_{i,\uparrow}^d - n_{i,\downarrow}^d) s_i^z \\
- h \sum_i (n_{i,\uparrow}^d - n_{i,\downarrow}^d) - h \sum_i s_i^z,
\]

(1)
where \(<i, j>\) means the nearest neighbor lattice sites \(i\) and \(j\), \(\sigma\) is a spin index, \(d_{i,\sigma}\) (\(d_{i,\sigma}^{\dagger}\)) is an annihilation (creation) operator, and \(n_{i,\sigma}^{d}\) is an occupation number of itinerant electrons. The on-site interaction between localized spins and itinerant electrons which reflects the Hund’s rule force is represented by the Ising-type coupling constant \(J\). The other parameters are: the hopping amplitude \(t\) (in the sequel we measure all energies in units of \(t\)) and the chemical potential \(\mu\).

In order to simulate various dopings of the \(d\)-electrons we allow for any value of their density, i.e. \(0 \leq \rho_d = \rho_{d\uparrow} + \rho_{d\downarrow} \leq 2\). Consequently, at a given site the \(d\)-electron occupancy \(n_d = n_{d,\uparrow} + n_{d,\downarrow}\) is assumed to be equal to 0, 1 or 2. So there are 2 states per site allowed for the spins (\(\uparrow\) and \(\downarrow\)) and 4 states per site allowed for the \(d\)-electrons (\(n_d = 0; n_{d,\uparrow} = 1\) and \(n_{d,\downarrow} = 0; n_{d,\uparrow} = 0\) and \(n_{d,\downarrow} = 1; n_d = 2\)).

The first two terms of the Hamiltonian (1) describe kinetic energy of the electrons in the ground canonical ensemble, the third one - on-site Hund interaction that couples localized spins and spins of itinerant electrons, and the last two terms represent energies of spins and electrons in an external magnetic field.

The localized spins play a role of an external potential for the electrons. This potential tunes its shape in such a way, that the total energy of the system attains its minimum. So there is a feedback between the subsystems of spins and electrons, and this is the feedback that is responsible for long-range arrangements of the spins.

Our purpose here is to examine how ground-state arrangements of the spins evolve when an external magnetic field \(h\) is applied. We solve the problem by constructing a restricted phase diagram of the model (1) within the configurational space, composed of all periodic phases (and their mixtures), for which the number of sites per unit cell is less or equal to 4. Then, for a chosen densities of electrons, we calculate magnetization of the electrons as a function of the magnetic field.

**II. METHOD OF CALCULATION**

Our trial set contains 12 periodic configurations of the spins. For each of them we perform the Fourier transformation of the Hamiltonian (1) and determine the electronic band structure of the conduction electrons. In other words, we solve the eigenvalue problem and find the eigenvalues \(E_{\nu\sigma}(k_x, k_y)\), with branch index \(\nu = 1, 2, ..., N_0 \leq 4\), spin index \(\sigma\) and the Bloch wavevector \(k = (k_x, k_y)\) (for more details see Refs.2,3). This requires us to diagonalize up to \(4 \times 4\) matrices and result in analytical formulae for at most 4 different energy bands, separately for spin-up and spin-down electrons.

In order to determine the ground-state energy we use a Brillouin zone grid of momentum points (typically \(100 \times 100\)) and sum eigenvalues of each band structure for each number of the conduction electrons. Then we construct the ground canonical phase diagram by direct comparing the Gibbs thermodynamical potentials of all phases from the trial set and selecting the lowest one. Next, we translate the grand-canonical diagram to the canonical phase diagram for arbitrary density \(\rho_d = \rho_{d\uparrow} + \rho_{d\downarrow}\) of the \(d\)-electrons. This procedure assures thermodynamical stability of all phases (both periodic and their mixtures) present in the resulting canonical phase diagrams4.

In the current study we repeat the calculations for a discrete set of values of the magnetic field \(h\), starting from 0 and up to \(h_{\text{max}} = 0.04\), with the steps equal to 0.002.
III. PHASE DIAGRAM

The phase diagram (Fig. 1) has been constructed within the restricted space for $J = 0.5$. Apart from the ferromagnetic (F) and the simplest antiferromagnetic (AF) we have found five other periodic phases in the diagram: two ferrimagnetic and three antiferromagnetic. All the phases, but one ferrimagnetic, are stable already at $h = 0$.

It is obvious that with an increase of the magnetic field $h$ antiferromagnetic phases become energetically less favorable than ferrimagnetic and ferrimagnetic less favorable than ferromagnetic. This general rule is also observed in our phase diagram, however, details of the phase transformations are not so evident. The simplest situation appears for electron densities close to 0 or 2, where the F phase is stable already for $h = 0$. The opposite limit is for $\rho_d \approx 1$, where the AF phase persists up to relatively high values of $h$, and then transforms into the F phase (the transition is not shown in the diagram).

More complex situation is observed for intermediate values of $\rho_d$, where either a ferrimagnetic or an antiferromagnetic phase is a ground state for $h = 0$. Then, even a tiny magnetic field $h$ is able to invoke a metamagnetic transition to the F phase, or a series of the transitions: first to a ferrimagnetic and then to the F phase (see Fig. 1,2).

IV. OTHER RESULTS AND CONCLUSIONS

The present studies show that even a tiny magnetic field can cause a substantial change of magnetic structure, especially for intermediate dopings. Although the range of densities $\rho_d$, where phases other than F and AF are ground states shrinks with an increase of $h$, some field induced arrangements (like one of the ferrimagnetic phases found in the present study) can appear on the diagram. It suggests that metamagnetic phase transitions are perhaps common phenomena in doped magnetic systems. Then, it would be interesting to verify experimentally the conjecture by examination properties of relevant solid solutions in magnetic fields.

A reorientation of the spins at the metamagnetic phase transitions are accompanied by jumps of magnetization of the electrons. However, the jumps are much smaller than the change of magnetization of the spins, as it can be noticed in Fig. 3, where the magnetization versus magnetic field for $J = 0.5$ and two different electron densities: $\rho_d = 0.3$, and $\rho_d = 0.55$ (i.e. along the red lines in Fig. 1) is shown.

It is also interesting that for some intervals of $h$ the magnetization of the electrons remains constant. It means that in this intervals the density of states of the electrons has energy gaps.

Let us finally mention that the phase diagram restricted to the lowest period phases provides only a crude information on the full diagram of the model, but we expect that this is the most essential information. The conjecture is justified by the results found previously for the spinless Falicov-Kimball model, where an increase in size of allowed unit cells does not produce significant qualitative changes in the phase diagram$^{2,3}$.

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FIGURES

FIG. 1. Phase diagram of the model for $J = 0.5$. Only the discret values of the magnetic field are taken into account: $h = 0.002p$, where $p = 0, 1, 2, ..., 20$. The horizontal straight line segments show electron density ranges inside which particular phases are stable. Different colours represent different phases: black - the ferromagnetic (F), red - the simplest antiferromagnetic (AF). All other phases are displayed in Fig. 2 (their colours are related to the colours of corresponding straight line segments). Blank gaps between the stright line segments indicate those density intervals in which macroscopic mixtures of two periodic phases have lower energy than any of them. The vertical red lines indicate electron densities $\rho_d = 0.3$ and $\rho_d = 0.55$, for which we calculated the magnetization of electrons as a function of the magnetic field (see Fig. 3).

FIG. 2. Arrangements of localized spins in phases represented in the phase diagram displayed in Fig. 1 (the background colours identify the phases on the diagram).

FIG. 3. Magnetization of the electrons versus magnetic field for $J = 0.5$ and two different electron densities: $\rho_d = 0.3$ (left panel) and $\rho_d = 0.55$ (right panel). Colours of the dots indicate stable arrangements of the localized spins (see captions to Fig.1 and 2 for explanations). The lines are only guides to eyes.