Model of magnetic ordering in coupled electron and spin systems

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Abstract. We present a simple model for a description of ground-state properties of itinerant electrons interacting with localized spins via an anisotropic spin-dependent local interaction ($J_z$) supplemented by the Ising interaction ($J_1$) between localized spins. The magnetic phase diagrams for both the itinerant electrons and the localized spins are analysed as functions of the spin-dependent interactions $J_z$ and $J_1$ as well as the total number of itinerant electrons ($N_d$). It is found that for both the ferromagnetic as well as antiferromagnetic Ising coupling $J_1$ various new types of spin orderings exhibiting a domain structure are generated. The strong correlations between magnetic phase diagrams of itinerant electron and spin subsystems are observed for $J_1 > 0$, while the coincidence is broken for $J_1 < 0$.

1. Introduction

The interplay between charge and spin degrees of freedom in strongly correlated systems has attracted an enormous interest in recent years due to the rich variety of charge and spin orderings found in some rare-earth and transition-metal compounds. Charge and spin superstructures have been observed, for example, in doped niclate [1], cuprate [2] and cobaltate [3] materials some of which constitute materials that exhibit high-temperature superconductivity. In order to describe both types of ordering in the unified picture, we proposed a model of localized spins and moving electrons on the square lattice, where the spins interact between themselves directly via the spin interaction of the Ising type, and both subsystems interact between themselves via an anisotropic spin-dependent local interaction. The model Hamiltonian is

$$H = \sum_{ij\sigma} t_{ij} d_{i\sigma}^\dagger d_{j\sigma} + J_z \sum_i (d_{i\uparrow}^\dagger d_{i\downarrow}^\dagger - d_{i\downarrow}^\dagger d_{i\uparrow}) S_i^z + J_1 \sum_{\langle ij \rangle} S_i^z S_j^z,$$

where $\langle ij \rangle$ means the nearest neighbour lattice sites $i$ and $j$, $\sigma = \uparrow, \downarrow$ is a spin index, $d_{i\sigma} (d_{i\sigma}^\dagger)$ is an annihilation (creation) operator of the itinerant electrons in the $d$-band Wannier state at site $i$. The first term of (1) is the kinetic energy corresponding to quantum-mechanical hopping of the itinerant $d$ electrons between sites $i$ and $j$. These intersite hopping transitions are described by the matrix elements $t_{ij}$, which are $-t$ if $i$ and $j$ are the nearest neighbours and zero otherwise (in the following all parameters are measured in units of $t$). The second term represents the anisotropic, spin-dependent local interaction of the Ising type between the localized spins and itinerant electrons that reflects the Hund’s rule. The third term describes the Ising interaction between the nearest neighbour spins.
2. Results and discussion

The main aim of this paper is to examine the ground-state properties of the model introduced above, with a special attention on the question how the additional interaction term, namely the Ising interaction $J_1$ between the nearest-neighbour localized spins, influences the ground-states of this two component model. We have investigated the model in the one dimensional case for a wide range of the Ising interaction $J_1 \in (-0.1, 0.1)$ with a step $\Delta J_1 = 0.01$. The ground states were studied by a well-controlled numerical method that we have elaborated [4, 5] for a description of the conventional Falicov-Kimball model. Later, the method was successfully used for various generalizations of the Falicov-Kimball model and different physical problems [6, 7]. This method is described in detail in our previous papers [4, 8].

To reveal the influence of $J_1$ on ground states we have started our study with the antiferromagnetic type of Ising interaction ($J_1 > 0$), where the magnetic phase diagrams in the $N_d - J_z$ plane have been calculated. A detailed analyse has been performed on the finite clusters up to $L = 32$ sites. To avoid an ambiguity in determination of the magnetic phases, specially the partially polarized (PP) and non polarized (NP) phases, we have examined the ground states only for even $N_d$. In the $J_z$ direction the calculations have been done with a step $\Delta J_z = 0.05$. Various phases that enter into the phase diagrams are classified according to $S^z = \sum_i (S_{1i}^z - S_{1i}^z)$ and $S_{d}^z = N_{d1}^z - N_{d1}^z$: the fully polarized (FP) phase is characterized by $|S^z| = L$, $|S_{d}^z| = N_{d}$, the partially polarized (PP) phases are characterized by $0 < |S^z| < L$, $0 < |S_{d}^z| < N_{d}$ and the non polarized (NP) phases are characterized by $|S^z| = 0$, $|S_{d}^z| = 0$.

In Figure 1 we summarize numerical results obtained for $J_1 = 0.05$. They represent typical examples of the magnetic phase diagrams in the positive $J_1$ limit. Comparing obtained results with $J_1 = 0$ counterpart (see Figure 2 and Ref. [6] for the complete list of ground-state configurations) we have found, that the increasing Ising interaction $J_1$ stabilizes the alternating NP phase ($\uparrow \downarrow \ldots \uparrow \downarrow$) for all $N_d$ in the region of small $J_z$ (bounded by the solid line in Figure 1), while the NP, PP and FP phases (with the same spin arrangements as were detected for $J_1 = 0$ and for given $N_d$) are shifted to higher values of $J_z$. Moreover, the antiferromagnetic Ising interaction $J_1$ generates new types of PP and NP phases. These new configurations are located in the lower part of the spin phase diagram, where for the model with $J_1 = 0$ only the FP configuration has been detected at the same model parameters. In Figure 1 the shaded area,
which determined the mentioned phases, is used for a better visualization. It is well known, that in the model where the spin interaction $J_1$ is omitted \[6\], the PP states represent the transition between the FP and NP states, and usually have the form of large ferromagnetic block combined with smaller antiparallel ferromagnetically ordered blocks. On the other hand, when the Ising interaction $J_1$ is switched on, these smaller blocks are replaced by the alternating type of ordering, where the PP configurations for $J_1 = 0.05$ have the form

$$
\begin{aligned}
    s_1 &= \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \\
    s_2 &= \uparrow \downarrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \\
    s_3 &= \uparrow \downarrow \uparrow \downarrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow
\end{aligned}
$$

(\text{the lower index denotes the number of consecutive sites occupied by up or down spins, or the number of repetitions of the block} [...] \) Similarly, the character of the new NP states is fully different in comparison to the case $J_1 = 0$, with evident influences of the Ising interaction. All configurations consist of $\uparrow \downarrow \downarrow$ blocks combined with larger ferromagnetically ordered clusters. The complete list of the new NP configurations detected for $J_1 = 0.05$ is shown in Table 1.

### Table 1. The new types of NP configurations determined for $J_1 = 0.05$ on $L = 32$.  

| $N_d$ | $s$ | $N_d$ | $s$ |
|------|-----|------|-----|
| 2    | $\uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow$ | 4    | $\uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow$ |
| 2    | $\uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow$ | 6    | $\uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow$ |
| 4    | $\uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow$ | 6    | $\uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow \downarrow \downarrow \uparrow$ |

It is very interesting, that all of these configurations have a special feature and namely, that for each spin distribution the cluster can be divided onto two equivalent parts with the mirror and spin flip arrangement. Comparing numerical results obtained for $|S^z|$ and $|S_d^z|$ one can find a nice correspondence between the magnetic phase diagrams of localized and itinerant subsystems. Indeed, with the exception of the new PP configurations, the corresponding FP, PP and NP phases perfectly coincide over the remaining part of diagrams. For the mentioned PP states the $d$-electron subsystem is either FP or PP.

For the ferromagnetic Ising interaction ($J_1 < 0$) it was observed a very similar scenario (Figure 3 illustrates the magnetic phase diagrams for $J_1 = -0.05$). As expected, the ferromagnetic interaction stabilizes the FP state, mainly for small $J_2$, while the remaining magnetic phases are gradually suppressed. Moreover, the ferromagnetic Ising interaction $J_1$...
generates the new types of PP and NP states, but contrary to $J_1 > 0$, they are observed for higher $d$-electron concentrations (usually for $N_d > L/2$). In Figure 3 the stability region of mentioned distributions is depicted by shaded area, which enlarges with decreasing $J_1$ towards to higher $N_d$ and smaller $J_z$. All new configurations determined for $J_1 = -0.05$ (laying in the shaded area) are listed in Table 2.

Table 2. The new types of NP and PP configurations determined for $J_1 = -0.05$ on $L = 32$.

| PP | 20 | 22 | 18 |
| NP | 18 | 18 | 18 |

Almost all NP phases have a “mirror symmetry”, but contrary to $J_1 > 0$ they are formed by antiparallel ferromagnetic domains. On the other hand, the PP configurations have a quasi-regular character, which are fully different from the $J_1 > 0$ or $J_1 = 0$ cases. In addition, the NP or PP configurations are also observed for small values of $J_z$ in isolated points or lines. Since their distribution depends strongly on the lattice size $L$, it is highly probable that the existence of these phases is a consequence of the finite size effects.

Comparing the $d$-electron magnetic phase diagram with its spin counterpart, there exists an evident difference. While the spin distributions (for $J_z$ small) are always FP, the $d$-electron subsystem can exhibit the FP, PP or NP behaviour. Taking into account the fact that the one-electron spectra of up-spin ($\epsilon_{i\uparrow}$) and down-spin ($\epsilon_{i\downarrow}$) electrons corresponding to the FP spin ordering are simply given by $\epsilon_{i\uparrow} = -2\cos(2\pi i/L) + J_z$, and $\epsilon_{i\downarrow} = -2\cos(2\pi i/L) - J_z$, one can show easily that the NP ordering has to disappear from the ground-state phase diagram in the thermodynamic limit. Thus only the FP states (for $N_d < N_d^c(J_z)$) and the PP states (for $N_d > N_d^c(J_z)$) can be the ground states of the model for small $J_z$.

2.1. Acknowledgments

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3. References

[1] C.H. Chen, S.W. Cheong, A.S. Cooper, Phys. Rev. Lett, 71, 2461 (1993)
[2] J.M. Tranquada, B.J. Sternlieb, J.D. Axe, Y. Nakamura, S. Uchida, Nature (London) 375, 561 (1995)
[3] K. Takada, H. Sakurai, E. Takayama-Muromachi, F. Izumi, Nature (London) 422, 53 (2003)
[4] P. Farkašovský, Eur. Phys. J. B 20, 209(2001)
[5] P. Farkašovský, Int. J. Mod. Phys. B 17, 4897 (2003)
[6] P. Farkašovský, H. Čencáriková, Eur. Phys. J. B 47, 517-526 (2005)
[7] P. Farkašovský, H. Čencáriková, N. Tomášovičová, Eur. Phys. J. B 45, 479 (2005)
[8] H. Čencáriková, P. Farkašovský, Int. J. Mod. Phys. B 18, 357 (2004)