Charge and spin orderings are studied on the simplest 1D and the 2D square lattice within the generalized Falicov-Kimball model with Hund coupling between localized and itinerant electrons. Using the restricted phase diagrams method (RPDM) a number of simple rules of formation of various sorts of ground state phases have been detected. In particular, relationships between density of current carriers (electrons or holes) and type of charge and magnetic arrangement has been determined. In 2D in the mixed valence regime only axial stripes (vertical or horizontal) have been found for intermediate values of the coupling constants. They are composed of ferromagnetic or antiferromagnetic chains interchanged with non-magnetic ones. For band fillings close to the half filling stripe phases oriented along one of the main diagonal direction are formed. The results suggest a possibility of tuning modulations of charge and magnetic superstructures with a change of doping.

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I. INTRODUCTION

Charge and magnetic superstructures observed in many transition metal oxides, as e.g. in $R_{2-x}Sr_xNiO_4$, where $R = La, Nd$, have stimulated an intensive search for explanation of origins of the phenomenon and its impact on physical properties of the systems. The subject has been analyzed primarily in the framework of various versions of the Hubbard or $t$-$J$ model. An important role of the Hund coupling in explaining magnetic properties of correlated electron systems was raised, e.g. in Refs. 13,14,15, and specifically in applying to the FKM, in Ref. 16. In fact, the model we deal with is very similar to the ferromagnetic Kondo lattice model, that was also considered in the context of charge and magnetic superstructures in correlated electron systems.

Here we assume the simplest Ising-type anisotropy of the Hund coupling what enables us to examine the model rigorously. The anisotropy is relevant in systems, where spin flip processes have a minor meaning and stable magnetically ordered phases occur (for more arguments see Refs. 19).

The extended model is still oversimplified to describe all details of real materials. But, since it comprises only basic interactions, that are present in all materials, where both localized and itinerant electrons are relevant, we expect that its characteristics emerging from our calculations are quite universal. Our expectations are justified by the fact, that phases similar to those we detected were also found by other authors studying different models and using quite different methods, as it was reported e.g. in Ref. 5 for a version of the Hubbard model and in Refs. 14,17 for the ferromagnetic Kondo (or Hund) lattice model.

In Ref. 12, only some basic properties of the model in 2D were examined. Farkašovký and Čenčariková studied the model by means of the small-cluster exact-diagonalization calculations and an efficient numerical method for large clusters containing up to 64 lattice sites. They constructed phase diagrams, where they found a number of various types of charge and spin distributions, and observed a gradual reduction of the stability region of the non-polarized (NP) phase in favor of the fully-polarized (FP) and partially polarized (PP) phases with an increase of the Hund coupling and with an increase in the number of localized particles. The studies are interesting, as they enable to examine the model in a complementary way, but the obtained results are too general for making predictions on details of charge and spin ordering for a given set of model parameters. Besides, there are some strange irregularities in their diagrams. For example, for small Hund couplings or for small densities of both localized and itinerant particles, one can find the FP phase at some isolated positions, surrounded by NP phases. And a lack of PP phases in a wide region.
of the diagram close to the chessboard AF phase, especially for small \( J \), seems to be an artefact resultant from taking into considerations only clusters with even numbers of sites.

A need for a clarification of this picture pushes us to examine the model more carefully. In our previous work we considered only 2D case and we used too small configurational space to detect many regularities. We merely noticed a few general tendencies for a formation of charge and/or spin ordered phases. Here we expand upon our preceding work both to 1D and 2D systems and provide a thorough analysis of the ground state phase diagrams using a much larger set of admissible configurations. It allows us to notice some simple rules of formation of periodic phases (as well as their mixtures) not noticed in previous studies.

The model Hamiltonian is

\[
H = t \sum_{\langle i,j \rangle} \sum_{\sigma=\uparrow,\downarrow} n_{i,\sigma}^d(\sigma) + \sum_i \sum_{\sigma,\eta=\uparrow,\downarrow} n_{i,\sigma}^d n_{i,\eta}^f - J \sum_i (n_{i,\uparrow}^d - n_{i,\downarrow}^d) (n_{i,\uparrow}^f - n_{i,\downarrow}^f),
\]

where \( \langle i,j \rangle \) denotes the nearest neighbor lattice sites \( i \) and \( j \), \( \sigma \) and \( \eta \) are spin indices, \( d_{i,\sigma} \) (\( d_{i,\sigma}^\dagger \)) is an annihilation (creation) operator, and \( n_{i,\sigma}^d \) (\( n_{i,\eta}^f \)) is an occupation number of itinerant (localized) electrons. The on-site interaction between localized and itinerant electrons is represented by two coupling constants: \( U \), which is spin-independent Coulomb-type and \( J \), which is spin-dependent and reflects the Hund’s rule force. The hopping amplitude \( t \) is set equal to one, so we measure all energies in units of \( t \).

Double occupancy of the localized electrons is forbidden, implying the on-site Coulomb repulsion \( U_{ff} \) between two \( f \)-electrons is infinite. Consequently, at a given site the \( f \)-electron occupancy is assumed to be \( n_f = n_{f,\uparrow} + n_{f,\downarrow} \leq 1 \) and the \( d \)-electron occupancy to be \( n_d = n_{d,\uparrow} + n_{d,\downarrow} \leq 2 \). So there are 3 states per site allowed for the \( f \)-electrons \( (n_f = 0; n_{f,\uparrow} = 1 \text{ and } n_{f,\downarrow} = 0; n_{f,\uparrow} = 0 \text{ and } n_{f,\downarrow} = 1) \) and 4 states per site allowed for the \( d \)-electrons \( (n_d = 0; n_{d,\uparrow} = 1 \text{ and } n_{d,\downarrow} = 0; n_{d,\uparrow} = 0 \text{ and } n_{d,\downarrow} = 1; n_d = 2) \).

All single-ion interactions included in Eq. (1) preserve states of localized electrons, i.e. the itinerant electrons traveling through the lattice change neither occupation numbers nor spins of the localized ones. Then \([H, f_{i,\sigma}^f f_{i,\eta}^f] = 0\) for all \( i \) and \( \eta \), so the local occupation number is conserved.

The localized electrons play the role of an external, charge and spin dependent potential for the itinerant electrons. This external potential is ”adjusted” by annealing, so the total energy of the system attains its minimum. In other words, there is a feedback between the subsystems of localized and itinerant electrons, and this is the feedback that is responsible for the long-period ordered arrangements of the localized electrons, and consequently for the formation of various charge and/or spin distributions at low temperatures.

In the next section we shortly describe our calculation scheme, then, in the third section we present two kinds of phase diagrams referring to pure magnets (section A) and diluted magnets (section B). The last section contains summary and discussion.

### II. THE RESTRICTED PHASE DIAGRAMS METHOD (RPDM)

We used RPDM first in our studies of the spinless 1D FKM in Refs.\(^{20,21}\) and then also in Refs.\(^{10,12,21}\). Within the method, calculations are performed for infinite systems but with a restriction to periodic phases, with periods not exceeded a certain value and their mixtures. Then, we can investigate both periodic phases and phase separation and segregation.

We emphasize that the RPDM is by no means a mean field approach and the calculations refer to infinite systems, not to finite clusters. So we do not need to deal with neither boundary nor finite size effects. Energies (per site) of all phases we consider here are evaluated with a very high and controllable accuracy. For small period phases with no more than 4 lattice sites in an unit cell energy bands are given by analytical expressions\(^{22}\), and the precision is limited merely by a selection of a grid in the \( k \)-space. For large period phases some very small errors, resulting from numerical diagonalization of matrices of size of the number of lattice sites in an unit cells may additionally enter. The details of the current work are as follows.

We performed calculations in 1D and 2D (the square lattice) for \( U = 1, 2, 4, 6, 8 \) and \( J \) changing from 0.2 up to 0.75\( U \) and within the configurational space restricted to all periodic phases with unit cells containing up to 12 lattice sites for pure magnets and up to 8 for diluted magnets.

To assure stability of the phases appearing on the diagrams, we constructed the grand canonical phase diagrams first (see Refs.\(^{20,21}\) for more detailed discussion of the stability issue) in the plane of the chemical potentials. Then we transformed the diagrams into the canonical phase diagrams in the plane of densities of localized \( (\rho_f) \) and itinerant \( (\rho_d) \) electrons. By applying this procedure one automatically includes all mixtures of the phases. The resulting phase
In order to calculate the Gibbs thermodynamic potential, we first determined the electronic band structure for the itinerant electrons for each candidate periodic phase. We employed a sufficiently tiny grid in the Brillouin zone (up to \( N_0 = 100 \) momentum points in 1D and up to \( N_0 = 80 \times 80 \) in 2D for each bandstructure). This required us to diagonalize up to \( 12 \times 12 \) matrices in the pure magnet case and up to \( 8 \times 8 \) matrices in the diluted magnet case at each discrete momentum point in the Brillouin zone and results in at most 12 and 8 different energy bands in pure and diluted magnet case, respectively. Hence, our calculations can be viewed as finite size but very large cluster calculations with cluster sizes ranging in 1D from \( N = 100 \) up to \( N = 100 \times 12 \) in the pure magnet and from \( N = 100 \) up to \( N = 100 \times 8 \) in the diluted magnet case, whereas in 2D from \( N = 80 \times 80 \) up to \( N = 80 \times 80 \times 12 \) in the pure magnet and from \( N = 80 \times 80 \) up to \( N = 80 \times 80 \times 8 \) in the diluted magnet case, depending on the number of sites in the unit cell \( (N = N_0 \cdot C \), where \( N_0 \) is equal to the number of unit cells and \( C \) denotes a number of lattice sites in unit cell for a given configuration of localized electrons). We performed all the calculations separately for spin up and down itinerant electrons. The eigenvalues of the band structure are summed up to determine the ground-state energy for each density of the electrons. Then, the Gibbs thermodynamical potential for a given configuration \( \{w_f\} \) is calculated for all possible values of the chemical potentials \( \mu_d \) and \( \mu_f \) of the conduction and localized electrons, respectively, through the formula

\[
G_{\{w_f\}} = \frac{1}{N} \sum_{\varepsilon_i, \varepsilon_j < \mu_d} (\varepsilon_i(\{w_f\}) + \varepsilon_j(\{w_f\})) - \mu_d(\rho_d + \rho_f) - \mu_f(\rho_f + \rho_f) \tag{2}
\]

where the symbol \( \varepsilon_i(\{w_f\}) \) \( \varepsilon_j(\{w_f\}) \) denotes energy eigenvalues of a band structure attributed to spin up (down) itinerant electrons for a given configuration \( \{w_f\} \) of localized electrons.

It appears that only a small part of the initial candidate phases can be found in the ground-state phase diagram. The actual number depends on \( U, J \) and \( C \) but the rate drops drastically with an increase of \( C \). We find that for the values of the parameters we considered it is less than 10\% in 1D and less than 2\% in 2D case.

## III. PHASE DIAGRAMS

In this paper we present two types of the ground-state phase diagrams. The first type (pure magnets) demonstrates only magnetic order, as it corresponds to the case \( \rho_f = 1 \) (each site is occupied by exactly one \( f\)-electron) in the plane \( (J, \rho_d) \). And the second type (diluted magnets) demonstrates both a magnetic and charge order in the plane \( (\rho_d, \rho_f) \) for fixed values \( J \) and \( U \). The diagrams show ground state configurations of the \( f\)-electrons both in 1D and 2D for representative values of the model parameters. For a pure magnet we selected \( U = 4, 0.2 \leq J \leq 3.0 \) in 1D and \( U = 6, 0.2 \leq J \leq 3.0 \) in 2D. And for the diluted magnet \( U = 2, J = 0.5 \) in 1D and \( U = 4, J = 0.5 \) in the 2D.

### A. pure magnets

In the pure magnetic diagrams the ferromagnetic phase (F) is stable for \( \rho_d \) close to 0 or 2 and the region of the stability increases with \( J \), whereas along the line \( \rho_d = 1 \) (the half-filling) the simplest AF phase is stable. Now, the most interesting story concerns a way of transforming between the two extreme phases with a change of \( \rho_d \).

Obviously, the process depends on \( J \), but it is the density \( \rho_d \) that plays a crucial role in determining a spin order. Namely, if \( \rho_d = p/q \), where \( p \) and \( q \) are relative prime numbers, then the period \( r \) of a stable phase in 1D is equal to \( q \) or a multiple of \( q \) (i.e. \( r = nq, n = 1, 2, \ldots \)). Consequently, if \( r = q \) and \( q \) is an odd number, then the system cannot be an antiferromagnetic (AF), but ferrimagnetic (FI). Indeed, we observe both FI and AF phases distributed over the whole region between the F and the simplest AF phases. This is in contrast to the results reported in Ref.\(^{15}\), where many FI phases (named as partially polarized PP) were missed in 1D because only systems containing even numbers of lattice sites were taken into account. On the other hand, our AF phases are consistent with NP (non polarized) phases reported in Ref.\(^{15}\).

It appears that not only the period is determined by \( \rho_d \). We found a remarkable feature concerning the number \( L_f \) of changes of the \( f\)-electron spin orientation (from up to down or from down to up) calculated per site. If in the diagram displayed in Fig. 1 we move up along a vertical line (i.e. when \( J \) is fixed) then \( L_f \) of subsequent phases increases with the density \( \rho_d \). What is more, for \( J \leq 1 \) in almost all cases \( L_f = \rho_d \). Then the number of itinerant electrons is equal to the number of pairs of localized electrons with magnetic moments oriented oppositely.

Physically this rule means that each moving electron is somehow associated with an exactly one abrupt change of the potential resulting from the localized electrons. In other words, the minimum energy is attained when the number
of moving electrons and the number of changes of the potential acting on them are equal to each other. The rule can be noticed by direct inspection, e. g. looking along the dashed line in Fig. 1 (for $J = 0.4$). In this case unit cells of phases located between F and the simplest AF phases are displayed in Table I.

![Diagram](image)

**FIG. 1:** The one-dimensional pure magnetic phase diagram restricted to all periodic phases with $\rho_f = 1$ and with the maximum period $C \leq 12$. Straight line segments mark stability intervals of the phases. Unit cells of the phases are expressed by sequences of the plus and minus signs placed close to (in almost all cases just above) the corresponding line segments. The signs “+” and “-” denote up and down spins of the $f$-electrons, respectively. The extended area below the curve line at the bottom of the diagram shows a stability region of the ferromagnetic phase F. Unit cells of phases located along the dashed vertical line for $J = 0.4$ are displayed in Table I.

| unit cell | $\rho_d$ | unit cell | $\rho_d$ | unit cell | $\rho_d$ |
|-----------|---------|-----------|---------|-----------|---------|
| $++-++-+--$ | 1/3      | $++-++-++-++$ | 4/11    | $++-++-++$ | 2/5     |
| $++-++-+--$ | 4/9      | $++-++-++-++$ | 3/5     | $++-++-++$ | 2/3     |
| $++-++-+--$ | 8/11     | $++-++-++-++$ | 3/4     | $++-++-++$ | 4/5     |
| $++-++-+--$ | 5/6      | $++-++-++-++$ | 6/7     | $++-++-++-++$ | 8/9 |
| $++-++-+--$ | 10/11    | $++-++-++-++$ | 1      |

**TABLE I:** Unit cells of phases located along the dashed line $J = 0.4$ in Fig. 1 and electron densities $\rho_d(= L_f)$ corresponding to them.

Obviously, for small enough $\rho_d$, where the F phase is stable, one has $L_f = 0$ and for $\rho_d = 1$, where the simplest AF phase is stable, one has $L_f = 1$. So it is clear that in 1D the density of itinerant electrons $\rho_d$ determines not only a periodicity (within an accuracy to a small natural number multiplier) of arrangement of the $f$-electrons but also strongly influences a relative distribution of spins up and down inside unit cells.

In 2D the process of transformation from F to AF with an increase of $\rho_d$ can be divided into two stages (see Fig. 2). First, anisotropic quasi-one-dimensional structures composed of parallel ferromagnetic chains oriented along one of the main lattice axis are formed. We call the area the region of axial stripes with ferromagnetic chains (see Figs. 2 and 3). For $J \leq 3.05$ this region ends up with the simplest phase belonging to this class, that is composed of ferromagnetic chains with alternating spin direction. In our considerations this is the very special phase, as it can be also viewed as composed of the simplest antiferromagnetic chains along the perpendicular axis. This is why we call the phase AF-f/a, to underline that it is the antiferromagnetic phase composed of ferro-/antiferro- magnetic chains (see Figs. 2 and 3).

Above the stability region of AF-f/a a majority of phases (see Fig. 3) are composed of either only the simplest antiferromagnetic chains (for $J \leq 1.2$) or with an admixture of ferromagnetic chains (for $J \geq 1.8$) and in the
intermediate interval of $1.2 \lesssim J \lesssim 1.8$ also of ferrimagnetic chains. Some phases found in this region can be viewed as composed of diagonal ferromagnetic chains oriented along the diagonal $(1,1)$ direction. And the final stage of the transformation of the phases with an increase of $\rho_d$ is the simplest AF phase with antiferromagnetic chains located along the both main lattice axes.

It appears that the transformation from F to the simplest AF phase is accompanied with an increase of a rate of localization of itinerant electrons, as with an increase of $\rho_d$ a mobility of the $d$-electrons becomes more and more restricted when the half-filling is approached. For small $\rho_d$, where the F phase is stable, the $f$-electrons act on the $d$-electrons as an uniform, site independent external field that don’t disturb their movements. Then, in the region of axial stripes with ferromagnetic chains the $d$-electrons can move easily but only along these chains, as along the perpendicular direction an external potential (coming from the $f$-electrons) alternates by taking two different values $U + J$ and $U - J$ what causes scattering of the $d$-electrons.

The AF-f/a phase is an optimal one with respect to the transport of the $d$-electrons through the lattice but only along one direction. Maybe it is related to the optimum doping reported in some materials, when there is a balance between a density of current carriers and their mobility over the lattice. Obviously, one should be cautious when trying to relate the results obtained for such a simple model with situations observed in real materials, but it is interesting that the optimum doping observed here is attained for $\rho_d$ close to 0.5, what corresponds to the special case of quarter filling.

A further increase of $\rho_d$ causes a complete vanish of ferromagnetic chains for small values of $J$ ($J \lesssim 1.2$) and a gradual decrease of their number for not too small $J$. It means that the $d$-electrons meet more and more potential barriers in any direction what makes them more and more localized. Obviously, the rate of localization becomes higher when $J$ is large.

Here we point out another interesting feature of the model. Namely, the critical value $\rho_d^*$ below which phases containing antiferromagnetic chains are stable increases with $J$, so the range of densities $\rho_d$ where the $d$-electrons become more localized shrinks, but at the same time a rate of the localization becomes more pronounced. It means that for large $J$ the $d$-electrons pass from a delocalized to localized regime within a relatively small interval of their densities. And the reported results suggest that in the limit of infinite $J$ the interval between the conducting F and insulating AF phase tends to zero (close to the line $\rho_d = 1$). This may be regarded as an analogy to the famous Nagaoka problem studied within the Hubbard model.
FIG. 3: Examples of ground-state periodic phases found in the diagram displayed in Fig. 2. The symbol ▲ (▽) denotes a spin up(down) f-electron. The shaded rectangulars in the left bottom parts of the pictures mark unit cells of the corresponding phases and the straight line segments mark the translation vectors.
B. diluted magnets

Let us now analyse a phase diagram corresponding to a diluted magnet, where both spin and charge orderings are relevant. The diagram is displayed in the \((\rho_f, \rho_d)\) plane for \(U = 2\) and \(J = 0.5\) in the 1D case (see Fig. 4) and for \(U = 4\) and \(J = 0.5\) in the 2D case (see Fig. 5). The maximum period \(C\) of allowed phases in the two cases is equal to 8. The values of the parameters \(U\) and \(J\) were chosen to be characteristic intermediate value representatives.

![FIG. 4: The canonical phase diagram of the extended FKM with Hund coupling for the 1D lattice and \(U = 2, J = 0.5\). The red crosses \(\times\) and horizontal straight line segments mark stability points or intervals of periodic phases. Their unit cells are drawn as sequences of small circles and plus and minus signs that correspond to sites non-occupied, occupied by the spin up and occupied by the spin down \(f\)-electrons, respectively.](image)

We found both in the 1D and 2D diagrams that a majority of periodic phases are located along one of the following three lines: \(\rho_f = 1 - \rho_d\), \(\rho_f = 2 - \rho_d\) or the diagonal \(\rho_f = 1 - \rho_d/2\). The first two mentioned lines correspond to mixed valence regimes.

Both antiferro- and ferrimagnetic arrangements of the \(f\)-electrons are found in the whole range of \(\rho_f\) and \(\rho_d\) in 1D and 2D. In 1D unit cells of phases located along the line \(\rho_f = 1 - \rho_d\) are composed of blocks of spins up (+) and down (−), whereas the pairs of opposite spins (+−) are stable along the \(\rho_f = 2 - \rho_d\) line. Unit cells of phases located along the diagonal \(\rho_f = 1 - \rho_d/2\) have the most homogeneous types of structures. A typical example of the transformation can be noticed e.g. for \(\rho_f = 2/3\), where the unit cell \(\{oo + + − −\}\) transforms first to \(\{o + o + o + o − \}\) and then to \(\{o + −\}\) for \(\rho_d = 1/3, 2/3\) and 4/3, respectively.

In 2D (see Figs. 5 and 6), phases located along the \(\rho_f = 1 - \rho_d\) line are composed of ferromagnetic (or diluted ferromagnetic) and nonmagnetic chains oriented along one of the lattice axis (e.g. D1 in Fig. 6). Phases belonging to this family are marked on the diagram in Fig. 5 by straight line segments. It means that they are stable over finite intervals of band fillings.

On the other hand, phases located along the \(\rho_f = 2 - \rho_d\) line are composed of antiferromagnetic and nonmagnetic chains. And phases located along the diagonal \(\rho_f = 1 - \rho_d/2\) can be viewed as composed of diluted ferro- or antiferromagnetic chains (D2, D3 and D4 in Fig. 6). The highest symmetry has the phase D3 placed at the central point of the diagram \((\rho_f = 1/2, \rho_d = 1)\).

It is interesting, that phases located along the diagonal \(\rho_f = 1 - \rho_d/2\) are insulating for any values of the model parameters we examined, as they have gaps at their Fermi levels, whereas phases found along the line \(\rho_f = 1 - \rho_d\) have no energy gaps at their Fermi levels. And phases located along the line \(\rho_f = 2 - \rho_d\) have no gaps for small values of \(U\), but they do have gaps for \(U\) large enough. This is consistent with the conjecture that the \(d\)-electrons can easily (i.e. without scattering) move along ferromagnetic and nonmagnetic chains, but along antiferromagnetic chains their mobility becomes suppressed.
FIG. 5: The canonical phase diagram of the extended FKM with Hund coupling for the 2D square lattice and \( U = 4, J = 0.5 \). The lines \( \rho_f = 1 - \rho_d \), \( \rho_f = 2 - \rho_d \), and \( \rho_f = 1 - \rho_d/2 \) are merely visual guides. The red crosses \( \times \) and horizontal straight line segments mark stability points and intervals of the periodic phases, respectively. Their unit cells are drawn as sequences of small circles and plus and minus signs that correspond to sites non-occupied, occupied by the spin up and occupied by the spin down \( f \)-electrons, respectively. A number of pairs of phases have the same unit cells but different translation vectors. Unit cells of the phases are displayed along the horizontal lines in the middle between the lines \( \rho_f = 1 - \rho_d \) and \( \rho_f = 1 - \rho_d/2 \), and in the middle between the lines \( \rho_f = 1 - \rho_d/2 \) and \( \rho_f = 2 - \rho_d \). The configurations located along the line \( \rho_f = 1 \) are presented in Fig. 3 and a set of characteristic configurations D1, D2, D3, D4, D5 is shown in Fig. 6.

FIG. 6: Characteristic ground state configurations displayed in Fig. 5. See the caption to Fig. 3 for more explanations.

### IV. SUMMARY AND DISCUSSION

Since the diagrams reported in this paper were constructed within the restricted space of periodic configurations, they can serve only as skeletons of the full diagrams. Here, similarly to what was found in the case of the simplest FKM, most of the diagrams areas are occupied by mixtures of various phases, occasionally penetrated by periodic phases.

With an increase of the maximum period \( C \) of admissible configurations more and more periodic phases with higher periods replace some of the mixtures on the canonical phase diagrams. However, we observed that the higher period phases do not destroy the diagrams’ structure, i.e. charge and spin distributions of these new phases follow the same rules that we already detected for low period phases. So our conjecture is that the full diagrams will be filled with phases of which charge and magnetic order can be easily predicted (for a given set of the coupling parameters and densities \( \rho_d \) and \( \rho_f \)). Of course, working within the RPDM we are not able to prove the statement rigorously, but since it appears to be quite reasonable, we expect that it can be established definitely by other methods.

In the limiting case of \( C \) tending to infinity not only periodic, but also aperiodic phases may happen to appear on the diagrams. It is not clear if some mixtures of low period phases survive in the central region of the full phases diagram. But it is quite possible, as in the simplest spinless FKM such phases are proven to have the lowest energy
in the large \( U \) limit\(^{22}\).

The rules of formation of the phases we detected from an analysis of the diagrams do not allow to determine unambiguously the ground state charge and spin arrangement for given values of \( \rho_f, \rho_d, U \) and \( J \), but they provide enough information needed for a rough prediction of what sorts of phases appear on the digrams and where they are located.

In the pure magnetic case (\( \rho_f = 1 \)) the F phase is stable for the densities \( \rho_d \) such that \( \rho_d < \rho_d^*(J) \) or \( 2 - \rho_d^*(J) < \rho_d \), where \( \rho_d^*(J) \) is an increasing function of \( J \). Within the interval of \( J \) ranging from 0.2 to 3.0 the function \( \rho_d^*(J) \) increases from about 0.2 to slightly above 0.6 in 1D (see Fig. 1) and from about 0.1 to around 0.55 in 2D (see Fig.2).

The results are consistent with the data obtained in Ref.\(^{18}\).

When \( \rho_d \) tends to the half filling \( \rho_d = 1 \), a transformation from F to the simplest AF phase occurs in 1D according to the following simple rules.

1. If \( \rho_d = p/q \), where \( p \) and \( q \) are relative prime integers, then if a phase is periodic, then its period is equal to \( nq \) (\( n = 1, 2, \ldots \)).

2. For \( J \) small and \( \rho_d = p/q \), with \( q \) being an even integer, periodic phases are antiferromagnetic, whereas for \( q \) being an odd number they are ferrimagnetic with the lowest possible magnetization; for large \( J \) higher magnetizations states become stable.

3. For a given \( J \) the number \( L_f \) of changes of spin orientation calculated per site increases with \( \rho_d \) and for small \( J \) it is equal to \( \rho_d \).

4. For a given density \( \rho_d \) the number \( L_f \) drops with an increase of \( J \).

The rules confirm a presence of quite well organized phase diagram structure not revealed in previous studies. In fact, some of the details shown in Ref.\(^{18}\) as, for example, arrangements of spins in a certain number of phases are in agreement with these rules. However, since only rings composed of even numbers of sites and even numbers of electrons were investigated in\(^{18}\) a number of FI phases were missed.

Driving mechanisms that are behind the detected rules are still not fully understood. Recently Brydon and Gulacsi\(^{19}\) discovered that competitive roles of the forward-scattering and back-scattering of itinerant electrons can explain observed richness of the spinless FKM diagrams. We hope that studies carried out along the similar ways could be also performed for the extended version of the FKM with the Hund coupling and elucidate the rules we observed.

In 2D the situation is more complex and we were not able to find out as many precise rules as in the 1D case. Even though, our phase diagram shows more regularities than those of reported in Ref.\(^{18}\). First of all, we noticed that all phases appeared in the diagram are composed of ferromagnetic or antiferromagnetic, and for intermediate values of \( J \) also ferrimagnetic chains parallel to each other. Obviously, the phases with only ferromagnetic chains have one-dimensional unit cells and they form axial stripes. These phases occur within an interval of electron densities \( \rho_d \) neighboring to those for which the F phase is stable. For \( J \leq 3.05 \) the interval ends with the simplest phase belonging to the family, the AF-f/a (ferromagnetic and antiferromagnetic) phase (see Fig. 2), that separates regions of axial stripes from those of containing antiferromagnetic chains (ferromagnetic and ferrimagnetic chains could be also present for not too small values of \( J \)).

So for \( \rho_d \) out of the stability regions of F, AF-f/a and axial stripes almost all phases are composed of either exclusively antiferromagnetic chains or with an admixture of ferromagnetic chains. Some of them containing only ferromagnetic chains are ferrimagnetic.

An analysis of diluted magnets diagrams (see Figs. 4-6) also permits us to fix some rules of charge and spin formation and its evolution with a change of the densities \( \rho_d \) and \( \rho_f \). Here we focused on the most representative three families of the phases. One of them consists of phases located along the main diagonal. This family corresponds to the most homogeneous phases relevant for the spinless FKM, and this is the only family of diluted periodic phases which is left in the limit of large \( U \) (if we keep \( J \) considerable smaller than \( U \)). Phases belonging to this family are characterized by the most uniform charge distribution but not necessarily the most uniform magnetic distribution. In 2D all but one particular phase have a form of sloped stripes composed of parallel lines of ferromagnetic chains (see conf. D2 and D4 in Fig. 6).

The only exception is the most symmetric, antiferromagnetic chessboard phase D3 placed in the center of the diagram. The phase has two-dimensional unit cell of size \( 2 \times 2 \) and is composed of diluted ferromagnetic lines (see Fig. 6).

Two other characteristic families refer to mixed valence regimes, for which either the condition \( \rho_d + \rho_f = 1 \) or \( \rho_d + \rho_f = 2 \) is fulfilled. These phases are ground states only for small and intermediate values of \( U \) (and \( U \gg J \)). In 1D, it appears that unit cells of phases belonging the first category (\( \rho_d + \rho_f = 1 \)) are built of blocks of spins up separated by pairs of empty sites from blocks of spins down. On the other hand, unit cells of phases belonging to the second category (\( \rho_d + \rho_f = 2 \)) consist of empty sites separated by pairs of oppositely oriented spins (\(+/-\)).

In 2D, all phases coming from the both mixed valence categories have the form of axial stripes. So they have the same type of charge ordering. Nevertheless their magnetic orders are clearly different, as phases that belong to the first class are composed of ferromagnetic chains (e.g. D1 in Fig. 6), whereas phases for which the condition \( \rho_d + \rho_f = 2 \)
is fulfilled are composed of antiferromagnetic chains (e.g. D5 in Fig. 6).

Our current studies confirm findings reported in Ref.\textsuperscript{2} that show that the compromise between kinetic energy of the \textit{d}-electrons and their interaction with the \textit{f}-electrons imposes formation of superstructures with shapes of stripes. Kinetic energy tends to spread out the \textit{d}-electrons uniformly over the lattice, but due to the presence of localized magnetic ions a kind of \textit{d}-electron density deformation must occur. Obviously, the deformation has to be conjugated with an arrangement of the \textit{f}-electrons. Apparently, the simplest departures from the homogeneity that are preferred have the form of axial or diagonal stripes.

Perhaps the most important conclusion emerging from this work is that the observed rules of formation of the phases suggest a possibility of manipulation of positional arrangements of magnetic ions diluted in the system and also their magnetic alignment with a change of doping. For example, one should be able to tune a modulation of charge and/or spin (stripes’ width). If it can be done in a controllable way, then in systems that can be described by the model it would be possible to change gradually an orientation of stripe phases (between axial and diagonal) and to change magnetic order along chains (from ferro- through ferri- up to antiferromagnetic).

We hope the results will motivate some new experimental work focusing on searching relationships between density of current carriers (electrons or holes) and observed charge and/or magnetic superstructure. According to our findings complicated ordering patterns should emerge from on-site interactions of localized and moving electrons and a simplified version of Hund’s rule. Therefore, we expect that experimental realizations of such patterns are robust in those correlated electron systems where a substantial anisotropy of spin-spin interactions occur.

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