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GROUND-STATES OF THE SPIN-ONE-HALF FALICOV-KIMBALL MODEL IN TWO DIMENSIONS[1]

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A combination of small-cluster exact-diagonalization calculations and a well-controlled approximative method is used to study the ground-states of the spin-one-half Falicov-Kimball model (FKM) in two dimensions. The results obtained are used to categorize the ground-state configurations according to common features for weak, intermediate and strong interactions. It is shown that only a few configuration types form the basic structure of the ground-state phase diagram. In particular, the largest regions of stability correspond to phase segregated/separated, n-molecular and axial striped configurations. This opens new route towards to understanding the inhomogeneous charge ordering in strongly correlated electron systems.

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1 Introduction

In the past decade, a considerable amount of effort has been devoted to understand the underlying physics that leads to an inhomogeneous charge stripe order in strongly correlated electron systems. The motivation was clearly due to the observation of a such ordering in doped nickelate and cuprate materials, some of which exhibit high-temperature superconductivity [1]. The Hubbard and $t-J$ models have been used the most frequently in the literature to study the problem of stripe formation [2, 3]. These studies showed on two possible explanations of formation the inhomogeneous spatial charge ordering. According to the first explanation the stripe phases arise from a competition between the tendency to phase separate (the natural tendency of system) and the long-range Coulomb interaction [2]. Contrary to this explanation, White and Scalapino proposed [3] a new mechanism that does not require the long-range interactions and according to which the charge stripe order arises from a competition between kinetic and exchange energies. Recently, it has been found by Lemanski et al. [4] that the spinless FKM (the simple model in

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which only the kinetic energy of itinerant electrons and the Coulomb interaction between the itinerant and localized electrons are taken into account [5]) exhibits the ground state with charge stripe order. In this paper we examine a generalized version of this model, the spin-one-half FKM, that represents a more realistic model for a description of the above mentioned materials. The Hamiltonian of the model can be written as the sum of three terms:

$$H = \sum_{ij\sigma} t_{ij} d^+_{i\sigma} d_{j\sigma} + U \sum_{i\sigma\sigma'} f^+_{i\sigma} f_{i\sigma} d^+_{i\sigma'} d_{i\sigma'} + \frac{U_{ff}}{2} \sum_{i\sigma} f^+_{i\sigma} f_{i\sigma} f^+_{i-\sigma} f_{i-\sigma}, \tag{1}$$

where $f^+_{i\sigma}$, $f_{i\sigma}$ are the creation and annihilation operators for an electron of spin σ in the localized state at lattice site i and $d^+_{i\sigma}$, $d_{i\sigma}$ are the creation and annihilation operators 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 neighbors and zero otherwise. The second term represents the on-site Coulomb interaction between the d-band electrons with density $n_d = N_d/L = \frac{1}{L}\sum_{i\sigma} d^+_{i\sigma} d_{i\sigma}$ and the localized f electrons with density $n_f = N_f/L = \frac{1}{L}\sum_{i\sigma} f^+_{i\sigma} f_{i\sigma}$, where L is the number of lattice sites. The last term represents the intra-atomic Coulomb interaction between the localized f electrons.

The full Hilbert space of the spin-one-half FKM is much larger than one of the spinless FKM and therefore numerical calculations are more complicated for the spin version of the model. Fortunately, the size of the Hilbert space can be reduced considerably in some special, but physically still very interesting limits, e.g., $U_{ff} \to \infty$. In the limit $U_{ff} \to \infty$ states with two f electrons at the same site are projected out thereby much larger clusters ($L \sim 36$) become accessible for the exact numerical studies in this reduced subspace. For this reason all calculations presented in this paper have been done at $U_{ff} = \infty$. The main goal for performing these calculations was to construct the comprehensive phase diagram of the spin-one-half FKM in two dimensions and on its base to try to answer the question on the possibility of the formation of inhomogeneous charge stripe order within this model.

Since the f-electron density operators $f^+_{i\sigma} f_{i\sigma}$ of each site i commute with the Hamiltonian (1), the f-electron occupation number is a good quantum number, taking only two values, $w_i = 0, 1$ according to whether the site i is unoccupied or occupied by the localized f electron (configurations with $w_i = 2$ are projected out due to $U_{ff} = \infty$). Therefore the Hamiltonian (1) can be replaced by $H = \sum_{ij\sigma} h_{ij} d^+_{i\sigma} d_{j\sigma}$ where $h_{ij} = t_{ij} + U w_i \delta_{ij}$.

Thus for a given f-electron configuration $w = \{w_1, w_2, \ldots, w_L\}$ the Hamiltonian H is the second-quantized version of the single-particle Hamiltonian $h(w)$, so the investigation of the model is reduced to the investigation of the spectrum of h for different configurations of f-electrons. This can be done in principle exactly (over the full set of f-electron configurations), or approximately (over an incomplete set). Here we use a combination of both methods. For clusters up to $L = 36$ we use small-cluster exact-diagonalization calculations and on larger clusters we adopt the well-controlled numerical method that we have developed recently to study ground states of the spinless FKM [6].

2 Results and discussion

To describe ground-states of the two-dimensional spin-one-half FKM we have performed an exhaustive numerical study of the model for a wide range of the Coulomb interaction ($U = 0.5, 1, 1.5 \ldots 8$). For each selected U all ground-state configurations corresponding to $N_f = 0, 1, .., L$ are calculated using methods mentioned above. To minimize the finite size effects the same procedure is repeated on several different clusters. Of course, such a procedure demands in practice a considerable amount of CPU time, which imposes severe restrictions on the size of clusters that can be studied within the numerical calculations ($L = 4 \times 4, 6 \times 6, 8 \times 8, 10 \times 10, 12 \times 12$). Fortunately, we have found that the main features of the phase diagram for weak, intermediate as well as strong interactions hold on all examined lattices and thus can be used satisfactorily to represent the behaviour of macroscopic systems. In particular, we have found that for each L there is a finite number of basic types of ground-state configurations that form the basic structure of the phase diagram. This structure depends only very weakly on the size of clusters and covers practically the whole area of the phase diagram in the $n_f - U$ plane. Let us start a discussion of the phase diagram with a description of configuration types that form its basic structure (see Fig. 1).

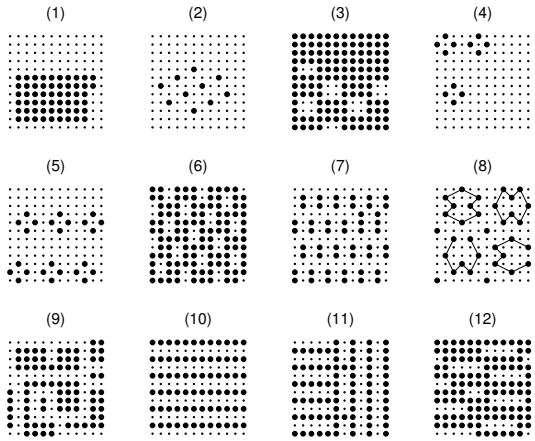

Fig. 1. Representative types of ground-state configurations that form the basic structure of the phase diagram in the $n_f - U$ plane. The large (small) dots correspond to occupied (vacant) sites.

(a) The segregated and phase separated phases (1,2). *(b) n-molecular phase separated phases* (3), that appear only in the weak coupling limit and n_f sufficiently large ($n_f \sim 0.9$). *(c) Four-molecular phases* (4,5). They are also stable only in the weak-coupling limit and according to n_f they prefer the four-molecular phase separated ($n_f < 0.2$) or the four-molecular regular ($n_f \sim 0.3$) distributions. *(d) Two-molecular phases* (6,7). This group consists of two subgroups. In the first subgroup ground states are the two-molecular regular distributions (only for $n_f > 1/2$), while in the second subgroup the ground states are the two-molecular ladders (only

for $n_f < 1/2$). *(e) The periodic phases* (8), detected in the very narrow region near $n_f = 0.2$ and U small. *(f) The labyrinth phases* (9). *(g) The axial stripes* (10-12).

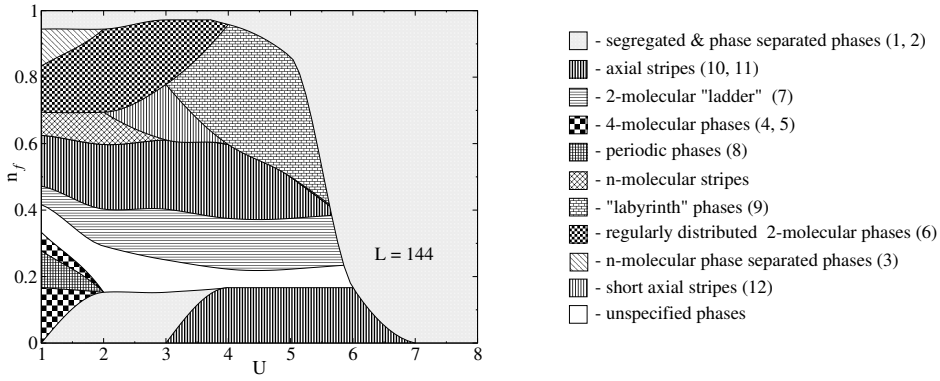

Fig. 2. The $n_f - U$ phase diagrams of the two-dimensional spin-one-half FKM at half-filling $n_f + n_d = 1$. The numbers in parentheses correspond to representative configurations from Fig. 1.

The stability regions of all above described phases are displayed in Fig. 2, where the comprehensive phase diagram of the two-dimensional spin-one-half FKM is presented in the $n_f - U$ plane. A direct comparison of these results with the one dimensional counterpart [7] shows that the basic structure of phase diagrams in one and two dimensions is very similar, and namely, in the central region of phase diagrams the prefered ground states are regular distributions while outside this region the prefered ground states are different types of phase separated and segregated phases. One can see that the largest regions of stability correspond to axial distributions of f electrons (the axial stripes, the labyrinth phases and two-molecular ladders). This is the main difference in comparison to the spinless FKM that prefers different type of diagonal distributions at half-filling band point $n_f + n_d = 1$. In the spin-one-half FKM the diagonal distributions are replaced by different types of axial stripe distributions. This opens new route towards to understanding the nature of stripe formations in strongly correlated electron systems.

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