Eur. Phys. J. B **20**, 209–215 (2001)

THE EUROPEAN PHYSICAL JOURNAL B

EDP Sciences

Ground-state properties of the Falicov-Kimball model in one and two dimensions

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Received 20 October 2000

Abstract. A new numerical method is used to study the ground-state properties of the spinless Falicov-Kimball model in one and two dimensions. The resultant solutions are used to examine the phase diagram of the model as well as possibilities for valence and metal-insulator transitions. In one dimension a comprehensive phase diagram of the model is presented. On the base of this phase diagram, the complete picture of valence and metal-insulator transitions is discussed. In two dimensions the structure of ground-state configurations is described for intermediate interactions between f and d electrons. In this region the phase separation and metal-insulator transitions are found at low f-electron concentrations. It is shown that valence transitions exhibit a staircase structure.

PACS. 75.10.Lp Band and itinerant models – 71.27.+a Strongly correlated electron systems; heavy fermions – 71.28.+d Narrow-band systems; intermediate-valence solids – 71.30.+h Metal-insulator transitions and other electronic transitions

1 Introduction

Valence and metal-insulator transitions are some of the most widely studied manifestations of cooperative phenomena in solids. These transitions are observed in a wide group of substances formed by transition-metal oxides as well as rare-earth sulfides and borides, when some external parameters (like pressure or temperature) are varied. They are in many cases first-order phase transitions, however, second-order transitions, ranging from very gradual to rather steep, are also observed [1].

To describe all such transitions in a unified picture, Falicov and Kimball [2] introduced a simple model in which only two relevant single-electron states are taken into account: extended Bloch waves and a set of localized states centered at the sites of the metallic ions in the crystal. It is assumed that insulator-metal transitions result from a change in the occupation numbers of these two sets of different electronic states, which remain themselves basically unchanged in their character. The Hamiltonian of the model can be written as the sum of three terms:

$$H = \sum_{ij} t_{ij} d_i^+ d_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_f \sum_i f_i^+ f_i, \quad (1)$$

where f_i^+, f_i are the creation and annihilation operators for an electron in the localized state at lattice site i with binding energy E_f and d_i^+, d_i are the creation and annihilation operators of the itinerant spinless electrons in the d-band Wannier state at site i.

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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 (in the following all parameters are measured in units of t). The second term represents the on-site Coulomb interaction between the d-band electrons with density $n_d = N_d/L = \frac{1}{L}\sum_i d_i^+ d_i$ and the localized f electrons with density $n_f = N_f/L = \frac{1}{L}\sum_i f_i^+ f_i$, where L is the number of lattice sites. The third term stands for the localized f electrons whose sharp energy level is E_f.

Since in this spinless version of the Falicov-Kimball model without hybridization the f-electron occupation number $f_i^+ f_i$ of each site i commutes with the Hamiltonian (1), the f-electron occupation number is a good quantum number, taking only two values: $w_i = 1$ or 0, according to whether or not the site i is occupied by the localized f electron.

Now the Hamiltonian (1) can be written as

$$H = \sum_{ij} h_{ij} d_i^+ d_j + E_f \sum_i w_i, \quad (2)$$

where $h_{ij}(w) = t_{ij} + U w_i \delta_{ij}$.

Thus for a given f-electron configuration $w = \{w_1, w_2 \dots w_L\}$ defined on the one or two-dimensional lattice with periodic boundary conditions, the Hamiltonian (2) is the second-quantized version of the single-particle Hamiltonian $h(w) = T + UW$, so the investigation of the model (2) is reduced to the investigation of the spectrum of h for different configurations of f electrons.

In spite of the fact that the Falicov-Kimball model is one of the simplest examples of interacting fermionic system, the theoretical picture of valence and insulator-metal transitions remains uncertain in the framework of this model. Even, in the existing literature on this model, different answers can be found on the fundamental question as to whether the Falicov-Kimball model can describe both the discontinuous and continuous changes of the f (d)-electron occupation number n_f (n_d) as a function of the f-level energy E_f [3]. It should be noted that this question is indeed crucial for the systems mentioned above, since, supposing [1] that the external pressure shifts the energy level E_f, the valence changes observed in some rare-earth and transition-metal compounds (SmS, SmB_6, Ti_2O_3, and so on) could be understandable purely electronic. Unfortunately, it was found that valence and insulator-metal transitions are very sensitive to the approximations used. Various approximations [3] (mean-field, virtual crystal, CPA, etc.) yield very different and often controversial results. This indicates that the study of valence and insulator-metal transitions may be successful only with methods which are relatively insensitive to the type of approximation used and, of course, with exact methods.

In our previous papers [4,5] we have showed that the method of extrapolation of small-cluster exact-diagonalization calculations can be very effective in describing the ground-state properties of the model, at least in some regions of the parameter space. Indeed, we have found that finite-size effects are practically negligible in the strong coupling limit and thus results obtained on relatively small clusters ($L < 30$) can be satisfactory extrapolated to the thermodynamics limit ($L \to \infty$). Using this method, the strong coupling phase diagram was described successfully, as well as the picture of valence and metal-insulator transitions in the 1d spinless Falicov-Kimball model [4]. It was found that for sufficiently large U the spinless Falicov-Kimball model undergoes only a few discrete intermediate-valence transitions. Thus, in the pressure-induced case, it can describe both the valence transitions from an integer-valence ground state ($n_f = 0$ or 1) into an inhomogeneous intermediate-valence ground state ($n_f \neq 0, 1$) and the transitions from one inhomogeneous intermediate-valence state with n_f into another inhomogeneous intermediate-valence state with $n'_f \neq n_f$.

However, the situation is more complicated for small and intermediate values of U since the finite-size effects are large in these regions for the clusters that can be studied using exact diagonalizations ($L < 30$). To obtain trustworthy results on the exact ground state of the Falicov-Kimball model in the weak coupling limit, one must examine much larger clusters ($L \sim 100$). Unfortunately, the clusters with $L > 30$ are beyond the reach of present day computers within exact diagonalizations and thus the only way is to compute the ground-state properties of the model by an approximate but well controlled method. Here we present one simple method based on a modification of the exact-diagonalization procedure used in our previous papers. First, we test this method for the case of the one-dimensional Falicov-Kimball model, and as a new result a comprehensive phase diagram of this model is presented. Then the method is used to study the ground states of the two dimensional Falicov-Kimball model which is still an open problem. (For a review on rigorous results concerning ground states of the two-dimensional Falicov-Kimball model see Ref. [6].) Our motivation for performing these calculations was to find and describe possible types of valence and metal-insulator transitions.

2 The method

The method used in this paper for the study of ground-state properties of the Falicov-Kimball model is a simple modification of the exact-diagonalization method [4,5] and consists of the following steps: (i) Chose a trial configuration $w = \{w_1, w_2 \dots w_L\}$. (ii) Having w, U and E_f fixed, find all eigenvalues λ_k of $h(w) = T + UW$. (iii) For a given $N_f = \sum_i w_i$ determine the ground-state energy $E(w) = \sum_{k=1}^{L-N_f} \lambda_k + E_f N_f$ of a particular f-electron configuration w by filling in the lowest $N_d = L - N_f$ one-electron levels (here we consider only the case $N_f + N_d = L$, which is the point of special interest for valence and metal-insulator transitions, caused by promotion of electrons from localized f orbitals ($f^n \to f^{n-1}$) to the conduction band states). (iv) Generate a new configuration w' by moving a randomly chosen electron to a new position which is chosen also at random. (v) Calculate the ground-state energy $E(w')$. If $E(w') < E(w)$ the new configuration is accepted, otherwise w' is rejected. Then the steps (ii)-(v) are repeated until the convergence (for a given U and E_f) is reached. Of course, one can move instead of one electron (in step (iv)) two or more electrons simultaneously. Thereby the convergence of method is improved. Repeating this procedure for different values of E_f and U one can immediately study the dependence of the f-electron occupation number $N_f = \sum_i w_i^{\min}$ on the f-level position E_f (valence transitions) or the phase diagram of the model in the E_f-U plane.

To test this method we have firstly studied the one-dimensional Falicov-Kimball model at half-filling, the ground state of which is well understood at present for both strong and weak interactions. In Table 1 we present results obtained using the numerical method described above for two representative values of U. In accordance with exact diagonalization results [4] we have found that the ground states of the Falicov-Kimball model at the half-filed band case are the most homogeneous configurations for sufficiently large values of U. It is interesting that although a relatively small number of iterations has been used in numerical simulations (typically 10 000 per site) the method was able to reproduce exactly the ground states for all examined cases. A comparison of numerically calculated results and those obtained using the exact diagonalization [5] is presented in Table 1, for $U = 0.6$. This shows that our method also reproduces exactly the ground states in the weak coupling region. This indicates that the method described above could be the convenient method for the study of valence and metal-insulator transitions since it is sufficiently accurate and sufficiently fast.

Table 1. The ground-states configurations of the one-dimensional Falicov-Kimball model calculated using the approximate method for $L = 30$ and two different values of U.

N_f	$U = 0.6$	$U = 8$
2	110000000000000000000000000000	100000000000000100000000000000
3	110000000100000000000000000000	100000000010000000001000000000
4	110000110000000000000000000000	100000001000000100000001000000
5	110001100001000000000000000000	100000100000100000100000100000
6	100001000010000100001000010000	100001000010000100001000010000
7	100010000100010001000100001000	100010000100010001000100001000
8	100010001001000100010001001000	100010001001000100010001001000
9	100100010010010001001001000100	100100010010010001001001000100
10	100100100100100100100100100100	100100100100100100100100100100
11	100101001001001010010010010100	100101001001001010010010010100
12	100101001010010100101001010010	100101001010010100101001010010
13	101001010100101010100101010010	101001010100101010100101010010
14	101010100101010101010100101010	101010100101010101010100101010
15	101010101010101010101010101010	101010101010101010101010101010

Indeed, while the results presented in Table 1 have been obtained within a few minutes, the corresponding calculations within exact diagonalizations (for a full set of f electron configurations) consumed several hundred hours of CPU time. Tests performed for a wide range of parameters of the model showed that clusters consisting of several hundred sites, are accessible for numerical studies using this method. For such large clusters the finite-size effects are considerably reduced, even in the weak coupling limit, and thus this method can be used successfully in the entire parameter space of the model. In Figure 1 we present the comprehensive phase diagram of the one-dimensional Falicov-Kimball model obtained using our method for $L = 240$. It is seen that our method reproduces correctly all the main results found by extrapolation of small-cluster exact-diagonalization calculations [4,5]. The largest phases in the phase diagram correspond to the periodic configurations with the smallest periods ($p < 9$) and the rational f-electron concentrations. The number of phases with the relevant width is strongly reduced with increasing U and thus only a few relevant phases (with $p \leq 5$) form the basic structure of the phase diagram in the strong coupling limit. A detailed analysis of the model performed for $U = 10$ ($L = 240$ and $L = 420$) showed that some of periodic phases with larger periods also persist in the strong-coupling regime, but their width is considerably smaller. A complete set of the phases (with width $w_{\rm D} > 10^{-10}$) that have been determined numerically as the ground states of the model for $U = 10$ is shown in Table 2. The valence transitions between these phases are discontinuous and of the type insulator-insulator, (there is a finite gap at the Fermi level for these phases) precisely as in the exact phase diagram. The phases with the smallest periods persist also in the weak coupling limit. In the regions of stability of these phases, the f-electron concentration number n_f is constant, while between these phases n_f changes continuously. In the inset we have also displayed the region of stability denoting the metallic phase

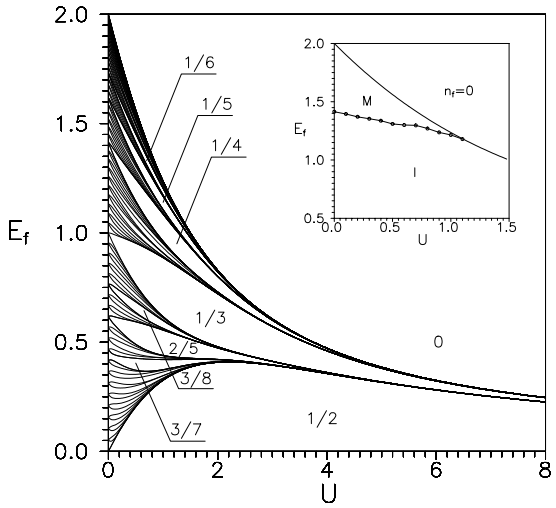

Fig. 1. The ground-state phase diagram of the one-dimensional Falicov-Kimball model in the E_f-U plane obtained for $L = 240$. All 120 phases corresponding to f-electron densities between $n_f = 0$ and $n_f = 1/2$ are displayed. The largest regions of stability correspond to the periodic configurations with the smallest periods and the rational f-electron densities: $n_f = 1/2, 3/7, 3/8, 2/5, 1/3, 1/4, 1/5, 1/6$ and $n_f = 0$. The inset shows the regions of stability for the metallic (M) and insulating (I) phase for $n_f > 0$.

corresponding to the phase separated configurations (only one part of the lattice is occupied by f-electrons while remaining one is free of f-electrons) which has been described only very roughly in the previous exact numerical studies [7]. Since the cluster used in our present study is sufficiently large, we suppose that the metallic phase as well as the whole phase diagram are described very well and thus the picture of valence and metal-insulator transitions is very close to real one. In the next section we present the corresponding picture of valence

Table 2. A complete set of phases (with width $w_{\rm D} > 10^{-10}$) which have been determined numerically as the ground states of the one-dimensional Falicov-Kimball model for $U = 10$. The empty configuration is stable for $E_f > 0.19804$.

n_f	$w_{\rm D}$
1/2	1.8712578×10^{-1}
1/3	1.0677360×10^{-2}
1/4	2.1048106×10^{-4}
2/5	2.1852806×10^{-5}
1/5	3.4509125×10^{-6}
2/7	1.1864030×10^{-8}
3/7	3.7646341×10^{-8}
1/6	5.0851783×10^{-8}
3/8	1.0913297×10^{-9}
1/7	$6.9578354 \times 10^{-10}$

and metal-insulator transitions for the two-dimensional Falicov-Kimball model.

3 Two-dimensional results

To show the basic structure of the phase diagram and to reveal the finite-size effects in two dimensions we have performed first the numerical calculations on small finite clusters of $L = 16$ and $L = 36$ sites. The results of numerical simulations are shown in Figure 2. For $L = 16$ we have also displayed the results of exact numerical diagonalizations which (see Fig. 2a) coincide with approximate results over the whole region of U and E_f values. This confirms that our method also works correctly in two dimensions. A direct comparison of one and two dimensional results shows that there are obvious similarities in the 1d and 2d phase diagrams. In both cases the largest regions of stability correspond to the fully occupied (empty) lattice $n_f = 1$ ($n_f = 0$) and the checkerboard configuration $n_f = 1/2$, with qualitatively the same shapes of phase boundaries. These phase boundaries are practically independent of the system size and thus the basic structure of the two dimensional phase diagram (corresponding to $n_f = 1$ and $n_f = 1/2$) can be extrapolated satisfactory to the thermodynamic limit $L \to \infty$. The remaining structure of the two dimensional phase diagram is, however, strongly influenced by finite size effects, especially in the weak coupling limit. Calculations performed for different sizes of clusters in the one and two dimensions, showed that finite-size effects (for $U \to 0$) are much larger for the 2d case. Obviously this is due to the fact that the ground states are highly degenerated in two dimensions. One can partially remove this deficiency by considering the periodic-antiperiodic boundary conditions (periodic in x and antiperiodic in y direction) instead of the periodic boundary conditions (used in our calculations), but unlike the 1d case, clusters of several hundred of sites are not sufficient to suppress the finite-size effects in two dimensions for $U \to 0$. This is illustrated in Figure 3 where

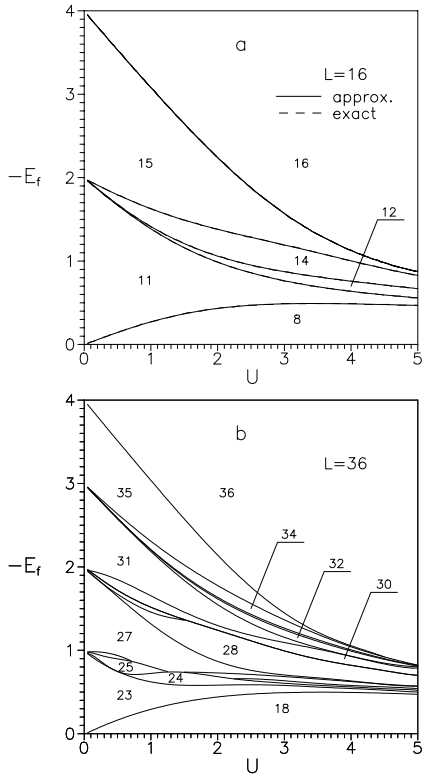

Fig. 2. The ground-state phase diagram of the two-dimensional Falicov-Kimball model in the E_f-U plane obtained for $L = 16$ (a) and $L = 36$ (b). All phases with finite regions of stability are displayed. The largest phases are denoted by corresponding f-electron numbers. The phase diagram for the region $n_f < 1/2$ can be determined by reflecting the region $n_f > 1/2$ in a mirror plane along the $E_f = 0$ axis and replacing n_f by $1 - n_f$.

the one and two dimensional results with different types of boundary conditions are plotted for $L = 400$ and $U = 0$. In the one-dimensional case the finite-size effects are negligible for $L = 400$, but they are still large in two dimensions for both periodic and periodic-antiperiodic boundary conditions. This indicates that one must consider clusters consisting of several thousand sites to suppress the finite-size effects for small U in two dimensions. Unfortunately, using our method only clusters consisting of several hundred lattice sites ($L \sim 400$) can be considered satisfactory, which is insufficient to present the correct results in the weak coupling limit. For this reason we did not continue in constructing the comprehensive phase diagram of the two-dimensional Falicov-Kimball model. Instead of this we concentrate our efforts to study the model at intermediate U, where it is expected that finite-size effects are considerably reduced. We do not discuss here the strong coupling limit of the model, since all ground-state configurations are insulating in this region [4] and thus there are no possibilities for insulator-metal transitions which were the motivation for our studies. A more complex situation is expected for intermediate values of U. To show the behavior of the two-dimensional Falicov-Kimball model in this region we have performed an exhaustive study of the

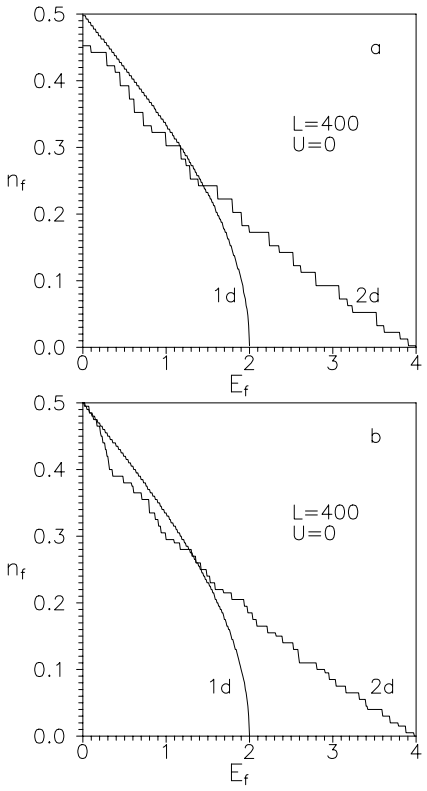

Fig. 3. Dependence of the f-electron occupation number n_f on the f-level position E_f for the periodic boundary conditions (a) and antiperiodic (periodic-antiperiodic) boundary conditions (b) in one dimension (two dimensions).

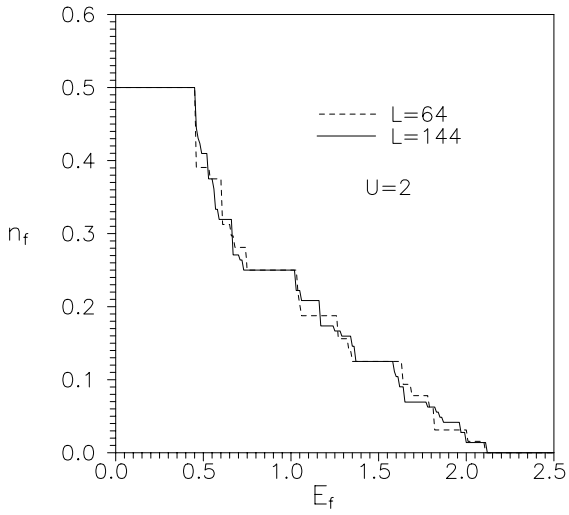

Fig. 4. Dependence of the f-electron occupation number n_f on the f-level position E_f calculated for $U = 2$ and two different clusters (8×8 and 12×12).

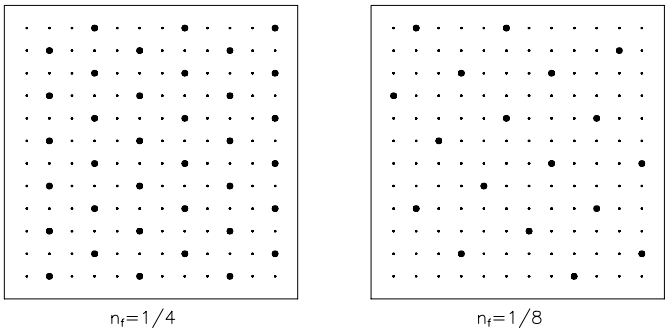

Fig. 5. The ground-state configurations of the two dimensional Falicov-Kimball model for $U = 2$ and two different f-electron densities: $n_f = 1/4$ and $n_f = 1/8$.

model at $U = 2$ on several different clusters. The results of numerical computations are summarized in Figure 4 where the f-electron density n_f is plotted as a function of the f-level position E_f for $L = 64$ and $L = 144$. Again there are obvious similarities to the one-dimensional case. The valence transitions have again a staircase structure, where one can easily recognize the primary structure which is almost independent of L (formed by configurations with $n_f = 1/2, 1/4, 1/8$), and the secondary structure depending strongly on L. Also the corresponding configurations that form the primary structure in the one and two dimensions are similar. In the one-dimensional case the primary structure is formed by the periodic configurations with the smallest periods, *i.e.*, {10...10} for $n_f = 1/2$, {100...100} for $n_f = 1/3$, {1000...1000} for $n_f = 1/4$, etc. The ground-state configurations that form the primary structure of the Falicov-Kimball model in two dimensions are displayed in Figure 5. In accordance with the exact results [8] we have found that the ground state of the Falicov-Kimball model at the half-filling band point ($n_f = 1/2$) is the checkerboard configuration. For $n_f = 1/4$ the ground state is periodic. It can be described as a periodic repetition of one occupied line (of slope 1/2) followed by three unoccupied lines. For large U this ground state was proved analytically by perturbation calculations [9]. Our results show that this type of the ground state persists also for intermediate values of U. For $n_f = 1/8$ a new type of the ground state configuration was found.

Let us now turn our attention to the problem of metal-insulator transitions in the two-dimensional Falicov-Kimball model. In Figure 6 we have displayed the dependence of the energy gap Δ at the Fermi level on the f-electron concentration [10]. It is seen that below some critical value of the f-electron concentration $n_{fc}(U)$ the energy gap is apparently suppressed and vanishes, probably discontinuously. Clearly this is demonstrated for larger values of U (see inset in Fig. 6). Thus we can conclude that the two-dimensional Falicov-Kimball model exhibits a discontinuous metal-insulator transition at $n_f = n_{fc}(U)$. In accordance with the one-dimensional case we suppose that this transition is the consequence of the phase separation which takes place for $n_f < n_{fc}(U)$. The numerical calculations performed on 8×8, 12×12, and 16×16 clusters fully confirmed our conjecture. In Figure 7 we have displayed the ground-states configurations found for several

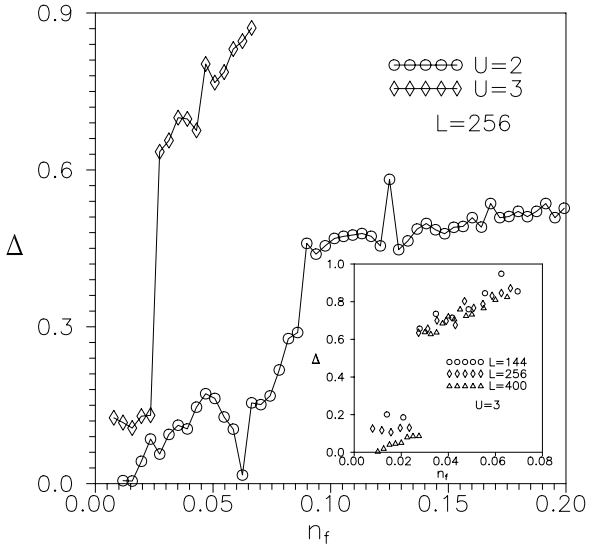

Fig. 6. Dependence of the energy gap Δ at the Fermi level on the f-electron density n_f for $L = 256$ and two different values of U. Inset: The behavior of Δ close to the insulator-metal transition point for several clusters (12×12, 16×16 and 20×20).

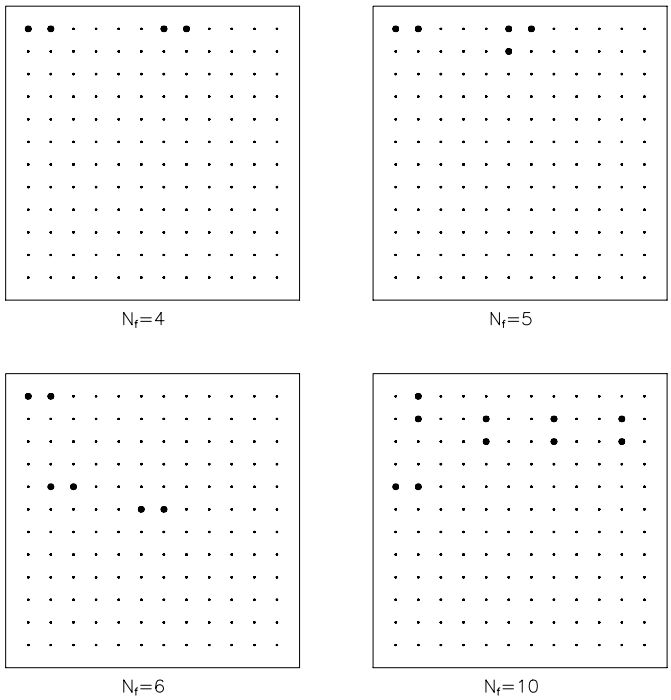

Fig. 7. The ground-state configurations of the two dimensional Falicov-Kimball model for $U = 2$ and several f-electron densities $n_f < n_{fc}$.

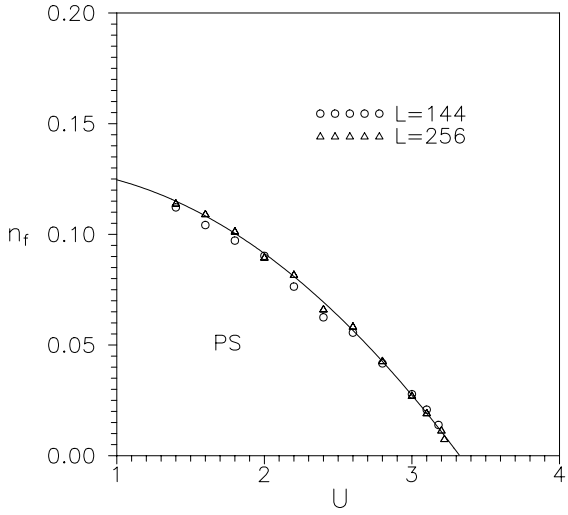

Fig. 8. The region of phase separation (PS) of the two-dimensional Falicov-Kimball model calculated for two different clusters (12×12 and 16×16).

f-electron concentrations less than n_{fc} on 12×12 cluster and $U = 2$. In all cases the ground state is phase separated, *i.e.*, f electrons occupy only one part of the lattice, while that remaining is free of f-electrons. The region of the phase separation in the n_f-U plane is shown in Figure 8. (Here we have displayed only results for $U > 1$ since in the opposite limit the finite-size effects are not negligible.) In comparison to the one-dimensional Falicov-Kimball model, where the phase separation takes place only for $U < t$, the two-dimensional model exhibits phase separation for values of U more than three times larger than t. Since the most interesting physics of the Falicov-Kimball model (the metal-insulator transition, and the phase separation) is connected with the existence of the phase separation domain, the fact that this domain persists also for $t < U$ is crucial for application of the model to rare-earth and transition-metal compounds. In these materials the values of the interaction constant U are much larger than the values of hopping integrals $t_{i,j}$ and thus for the correct description of valence and metal-insulator transitions in these compounds one has to take the limit $U > t$ and not $U < t$.

It should be noted that our numerical study of the two-dimensional Falicov-Kimball model represents one of the first attempts to find a complete set of the ground-state configurations for this model for intermediate interactions. Till now, there existed only a few numerical results for this region [11]. These results have been obtained for a restricted class of periodic configurations and thus they could not describe some of important features of the model, *e.g.*, the phase separation when the ground-state configurations are apparently not periodic (see Fig. 7). Finally, it should be noted that the applicability of our numerical method is much broader. Although we presented here results for one and two dimensions only, the method can be used directly for in three dimensions, at least for qualitative studies of the model. The study of relative models, like the spin-1/2 Falicov-Kimball model is also available within this method. Work in this direction is currently in progress.

In summary, a new numerical method was used to study the ground-state properties of the spinless Falicov-Kimball model in one and two dimensions. The results obtained were used to examine the phase diagram of the model and possibilities for valence and metal-insulator transitions. In the one dimension a comprehensive phase diagram as well as the picture of valence and metal-insulator transitions were described. As a new result we presented the region of stability for the metallic phase which was described only very roughly in the previous exact numerical studies. In two dimensions the structure of the ground-state configurations was described for intermediate interactions between f and d electrons. In this region the phase separation and metal-insulator transitions were found at low f-electron concentrations. It was shown that valence transitions exhibit a staircase structure.

This work was supported by the Slovak Grant Agency VEGA under grant No. 2/7021/20. Numerical results were obtained using computational resources of the Computing Centre of the Slovak Academy of Sciences.

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