Ground-state properties of the Falicov-Kimball model with correlated hopping in two dimensions

2002 J. Phys.: Condens. Matter 14 499

(http://iopscience.iop.org/0953-8984/14/3/318)

INSTITUTE OF PHYSICS PUBLISHING JOURNAL OF PHYSICS: CONDENSED MATTER

J. Phys.: Condens. Matter **14** (2002) 499–506 PII: S0953-8984(02)27348-8

Ground-state properties of the Falicov–Kimball model with correlated hopping in two dimensions

Pavol Farkašovský and Natália Hudáková

Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 043 53 Košice, Slovakia

Received 27 July 2001, in final form 28 September 2001
Published 21 December 2001
Online at stacks.iop.org/JPhysCM/14/499

Abstract

A new numerical method, recently developed to study ground states of the Falicov–Kimball model (FKM), is used to examine the effects of correlated hopping on the ground-state properties of this model in two dimensions. It is shown that the ground-state phase diagram as well as the picture of metal–insulator transitions found for the conventional FKM (without correlated hopping) are substantially changed when the correlated hopping term is added. The effect of correlated hopping is so strong that it can induce the insulator–metal transition, even in the strong-coupling limit, where the ground states of the conventional FKM are insulating for all f-electron densities.

1. Introduction

Since its introduction in 1969, the Falicov–Kimball model (FKM) [1] has become an important standard model for a description of correlated fermions on a lattice. The model was originally proposed to describe metal–insulator transitions and has since been investigated in connection with a variety of problems such as binary alloys [2], the formation of ionic crystals [3], and ordering in mixed-valence systems [4]. It is the latter language that we shall use here, considering a system of localized f electrons and itinerant d electrons coupled via the on-site Coulomb interaction U. The Hamiltonian of the spinless FKM is

$$H = \sum_{ij} t_{ij} d_i^+ d_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_{\mathrm{f}} \sum_i f_i^+ f_i \tag{1}$$

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 for an electron in the conduction band. The conduction band is generated by the hopping matrix elements t_{ij}, which describe intersite transitions between the sites i and j. Usually it is assumed that $t_{ij} = -t$ if i and j are nearest neighbours and $t_{ij} = 0$ otherwise (the conventional FKM); however, in what follows we consider a much more realistic type of hopping, so for the moment we leave it as arbitrary.

0953-8984/02/030499+08$30.00

Recent theoretical works based on exact numerical and analytical calculations showed that the FKM, in spite of its relative simplicity, can yield the correct physics for describing such fundamental phenomena as valence-change transitions, metal–insulator transitions, crystallization, charge ordering, etc. For example, it was found that the spinless FKM, in the pressure-induced case, can describe both types of intermediate-valence transition observed experimentally in rare-earth compounds: a discontinuous insulator–insulator transition for sufficiently strong interactions [5] and a discontinuous insulator–metal transition for weak interactions [6]. In addition, at non-zero temperatures this model is able to provide the qualitative explanation for the anomalous large values of the specific heat coefficient and for the extremely large changes of the electrical conductivity [7] found in some intermediate-valence compounds (e.g., in SmB_6). Moreover, very recently the spin-one-half version of the FKM has been used to describe a discontinuous intermediate-valence transition (accompanied by a discontinuous insulator–metal transition) in SmS [8] as well as for a description of an anomalous magnetic response of the Yb-based fluctuating-valence compounds [9].

On the other hand, it should be noted that the model Hamiltonian (1) neglects all non-local interaction terms, and thus it is questionable whether the above-mentioned results persist also in more realistic situations when non-local interactions will be turned on. An important non-local interaction term obviously absent in the conventional FKM is the term for correlated hopping, in which the d-electron hopping amplitudes between neighbouring lattice sites i and j depend explicitly on the occupancy ($f_i^+ f_i$) of the f-electron orbitals; i.e.,

$$\tilde{t}_{ij} = t_{ij} + t'_{ij}(f_i^+ f_i + f_j^+ f_j). \tag{2}$$

The importance of the correlated hopping term has already been mentioned by Hubbard [10]. Later Hirsch [11] pointed out that this term may be relevant in the explanation of superconducting properties of strongly correlated electrons. Here we examine effects of this term on ground-state properties of the two-dimensional FKM. The same subject has been studied recently by Wojtkiewicz and Lemanski [12]. To achieve compatibility with their results (one of goals of this paper is to re-examine these results), we do not consider here other non-local interactions, although, some of them (e.g., the intersite Coulomb interaction) are of the same order as the correlated hopping term. This will be dome in a future publication.

Thus the spinless FKM in which the effects of correlated hopping are included can be written as

$$H = \sum_{\langle ij \rangle} t_{ij} d_i^+ d_j + \sum_{\langle ij \rangle} t'_{ij}(f_i^+ f_i + f_j^+ f_j) d_i^+ d_j + U \sum_i f_i^+ f_i d_i^+ d_i + E_{\mathrm{f}} \sum_i f_i^+ f_i. \tag{3}$$

The first term of (3) is the kinetic energy corresponding to quantum mechanical hopping of the itinerant d electrons between the nearest-neighbour sites i and j. The second term is just the correlated hopping term discussed above. The third term describes the on-site Coulomb interaction between the d-band electrons with density $n_{\mathrm{d}} = (1/L)\sum_i d_i^+ d_i$ and the localized f electrons with density $n_{\mathrm{f}} = (1/L)\sum_i f_i^+ f_i$, where L is the number of lattice sites. The last term stands for the localized f electrons whose sharp energy level is E_{f}.

Since in this spinless version of the FKM without hybridization the f-electron occupation number $f_i^+ f_i$ of each site i commutes with the Hamiltonian (3), 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. Therefore the Hamiltonian (3) can be written as

$$H = \sum_{\langle ij \rangle} h_{ij}(w) d_i^+ d_j + E_{\mathrm{f}} \sum_i w_i \tag{4}$$

where $h_{ij}(w) = \tilde{t}_{ij}(w) + U w_i \delta_{ij}$ and

$$\tilde{t}_{ij}(w) = t_{ij} + t'_{ij}(w_i + w_j). \tag{5}$$

Thus for a given f-electron configuration $w = \{w_1, w_2, \ldots, w_L\}$ the Hamiltonian (4) is the second-quantized version of the single-particle Hamiltonian $h(w)$, so the investigation of the model (4) is reduced to the investigation of the spectrum of h for different configurations of f electrons. Since the d electrons do not interact among themselves, the numerical calculations should precede directly in the following steps.

(i) Having $w = \{w_1, w_2, \ldots, w_L\}$, U, E_f, and the nearest-neighbour hopping amplitudes t and t' fixed (in the following, $t = -1$, and all energies are measured in units of t), find all eigenvalues λ_k of $h(w)$.

(ii) For a given $N_f = \sum_i w_i$, determine the ground-state energy $E(w, U, E_f) = \sum_{k=1}^{N-N_f} \lambda_k + E_f N_f$ of a particular f-electron configuration w by filling in the lowest $N_d = N - N_f$ one-electron levels (here we consider only the case $N_f + N_d = L$, which is the point of the special interest for valence and metal–insulator transitions caused by promotion of electrons from localized f orbitals ($f^n \rightarrow f^{n-1}$) to the conduction band states).

(iii) Find the w^0 for which $E(w, U, E_f)$ has a minimum. Repeating this procedure for different values of U, t' and E_f, one can study directly the ground-state phase diagram and valence transitions (a dependence of the f-electron occupation number on the f-level position E_f) in the FKM with correlated hopping.

A direct application of this method has been used successfully in our previous papers [5,6] for the description of ground-state properties of the one-dimensional FKM model without correlated hopping ($t' = 0$). It was shown that finite-size effects are negligible for a wide range of the model parameters (e.g., strong interactions) and thus results obtained on relatively small clusters ($L < 30$) can be satisfactory extrapolated to the thermodynamic limit ($L \rightarrow \infty$). Using this method we have described satisfactorily the strong-coupling phase diagram as well as the picture of valence and metal–insulator transitions in the one-dimensional spinless FKM [5] with $t' = 0$. It was found that for sufficiently large U the spinless FKM undergoes only a few discrete intermediate-valence transitions. These intermediate-valence transitions are insulator–insulator transitions, since they are realized between the insulating ground states corresponding to the most homogeneous configurations, which are the ground states in this region [13]. Thus, there are no insulator–metal transitions in the 1D conventional FKM for strong interactions. In our next paper [14], we have shown that this picture of valence and metal–insulator transitions is dramatically changed if the term for correlated hopping is included. One of the most important results found for the one-dimensional FKM with correlated hopping was that the correlated hopping can induce the insulator–metal transition, even in the half-filled-band case $n_d = n_f = 1/2$ [15][1]. In this paper we try to show that the same result holds also for the two-dimensional case. Similar calculations are performed also away from the half-filled-band case with the goal of examining possibilities for metal–insulator transitions in the strong-coupling limit. Further inspiration for performing these calculations was provided by the recent paper of Wojtkiewicz and Lemanski [12], where the authors studied the two-dimensional FKM with correlated hopping using the combination of a perturbation expansion (up to the second order) and the method of restricted phase diagrams. They found that just a few phases form the ground-state phase diagram of the model in the strong-coupling limit. For example, the ground state of the model for $E_f = 0$ is the chessboard charge-density-wave (CDW) phase for all $0 < t' < 1$. Here we show that some other configurations (e.g., the segregated configuration) can also be ground states of the FKM at $E_f = 0$; thereby the ground-state phase diagram as well as the picture of metal–insulator transitions are substantially changed.

[1] Note that such a transition cannot be induced by long-range hopping.

2. The method

Since the number of configurations that should be examined to obtain the ground-state energy of the FKM grows exponentially with the system size, direct application of the exact-diagonalization method described above is restricted to clusters up to 30 sites. In our previous papers we showed that clusters of this size are sufficient to suppress finite-size effects in one dimension [5, 6]; however, to obtain reliable results on the ground-state energy of the model in two dimensions, one has to 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 to proceed is to compute the ground-state properties of the model by an approximate but well controlled method. Here we use the simple method based on a modification of the exact-diagonalization procedure described above. The method consists of the following steps:

(i) Chose a trial configuration $w = \{w_1, w_2, \ldots, w_L\}$.
(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.
(iv) Generate a new configuration w' by moving a randomly chosen electron to a new position which is also chosen 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 steps (ii)–(v) are repeated until convergence (for given parameters of the model) is reached. Of course, one can move instead of one electron (in step (iv)) two or more f electrons; the convergence of the method can thereby be improved. Indeed, tests that we have performed for a wide range of the model parameters showed that the latter implementation of the method, in which $N_0 > 1$ electrons (N_0 should be chosen at random) are moved to new positions, overcomes better the local minima of the ground-state energy. This also improves the accuracy of the method.

This method was first used in our recent paper [16] to study the ground-state properties of the one- and two-dimensional FKM without correlated hopping. It was found that for small and intermediate clusters ($L \sim 30$) the method is able to reproduce exactly the ground states of the conventional FKM, even after a relatively small number of iterations (typically 10 000 per site). For such clusters the method is only rarely stopped at the local minimum. Of course, with increasing L the problem of local minima appears often. Fortunately, it can be considerably reduced by using a more efficient algorithm (one is discussed above) or by increasing the number of iterations. The latter case, however, imposes severe restrictions on the size of clusters than can be studied with this method ($L \sim 100$, for 10^6 iterations per site). To verify the convergence of this method for the two-dimensional FKM with correlated hopping, we have performed the same calculations for a cluster of 4×4 sites, where ground states can be obtained also within exact-diagonalization calculations. Numerical results obtained for a wide range of the model parameters ($t' = -1, -0.8, \ldots, 1$, $U = 0, 0.1, \ldots, 10$) showed that the exact ground states can again be reproduced after $\sim$10 000 iterations per site.

3. Results and discussion

The most interesting question that arises for the FKM with correlated hopping is whether the correlated hopping term can change the ground-state phase diagram and the picture of valence

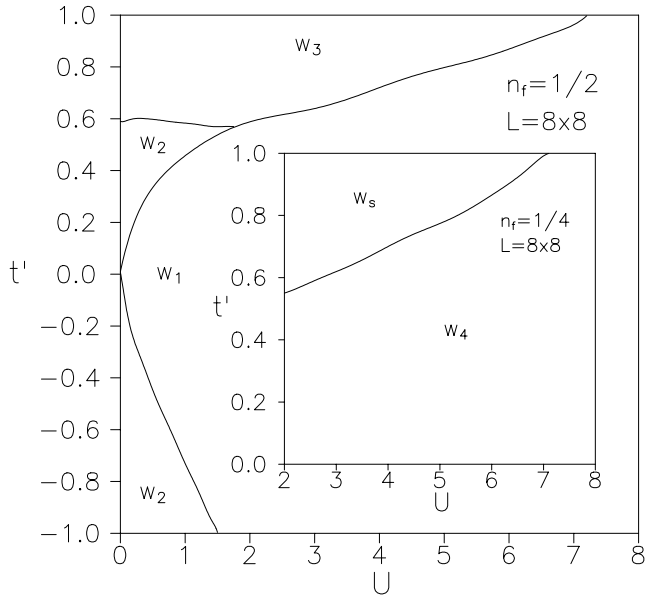

Figure 1. The t'–U phase diagram of the two-dimensional FKM with correlated hopping at half-filling ($E_f = 0, n_f = n_d = 0.5$). The three different phases correspond to the CDW state w_1, the configuration with alternating lines of occupied and unoccupied sites (w_2), and the segregated configuration w_3. The inset shows the t'–U phase diagram for $n_f = 1/4$ and $U > 2$. The two different phases correspond to the segregated configuration and the configuration w_4 that has been proven to be the ground state of the conventional FKM for large U.

and metal–insulator transitions found for the conventional FKM ($t = -1$ and $t' = 0$). The nature of the ground state, its energetic and structural properties, and the correlation-induced metal–insulator transitions are subjects of special interest. For the conventional FKM these problems are well understood at least in the symmetric case ($E_f = 0, n_f = n_d = 1/2$). In this case the localized f electrons fill up one of two sublattices of the hypercubic lattice (the CDW state), and the corresponding ground state is insulating for all $U > 0$. Thus, for finite interaction strength there is no correlation-induced metal–insulator transition in the symmetric case.

One can expect, on the basis of simple arguments, the ground-state phase diagram of the FKM with correlated hopping to be very different from one discussed above for the conventional FKM. Indeed, the following selection of hopping matrix amplitudes $t = -1$ and $t' > 0$ may favour the segregated configuration, since the itinerant d electrons have the lower kinetic energy in this state. This mechanism could lead, for example, to instability of the CDW state that is the ground state for $t' = 0$, and thereby to a metal–insulator transition, even in the symmetric case. To examine the possibilities for such a transition in two dimensions, we have performed an exhaustive study of the model on 6×6 and 8×8 clusters (with periodic boundary conditions) for a wide range of parameters t' and U. The results of numerical calculations are summarized in figure 1 in the form of the t'–U phase diagram. In addition to the CDW state w_1 that is the ground state at $t' = 0$ for all non-zero U, we found two new phases that can be ground states of the model—namely, the configuration with alternating lines of occupied and unoccupied sites w_2 and the segregated configuration w_3 (see figure 2). Thus at non-zero t' the CDW state w_1 becomes unstable against the transition to w_2 and w_3. The transition from w_1 to w_2, like that from w_1 to w_3, is a insulator–metal transition, since the configuration w_1 has

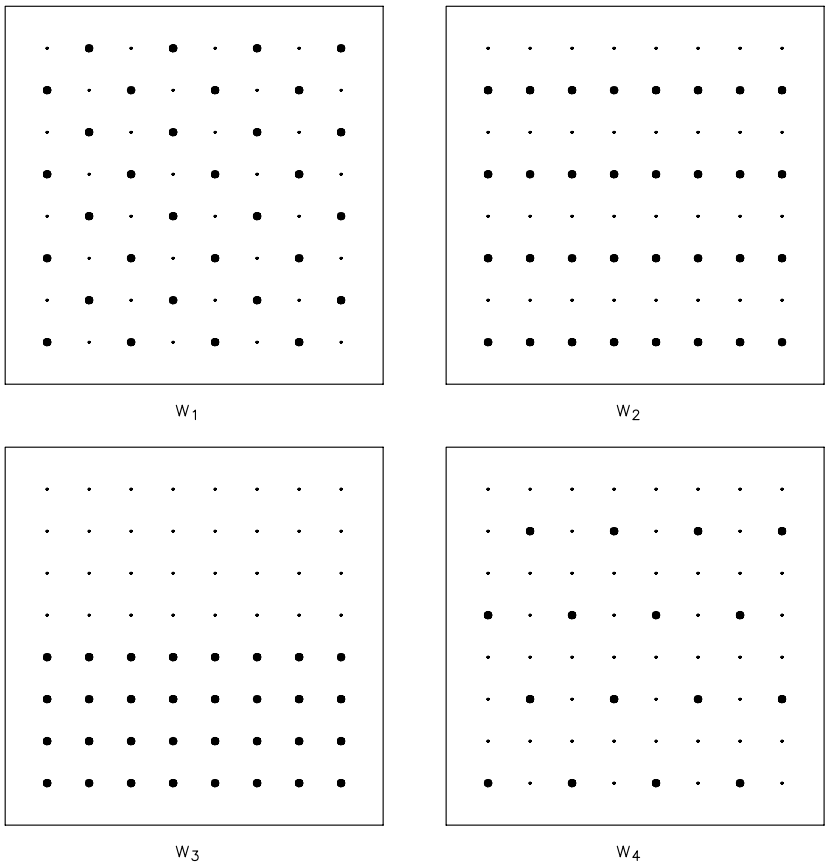

Figure 2. The ground-state configurations of the two-dimensional FKM with correlated hopping for $n_f = 1/2$ (w_1, w_2, and w_3) and $n_f = 1/4$ (w_4).

the finite gap ($\sim U$) at the Fermi energy[2] for all non-zero values of U, while both w_2 and w_3 are metallic in the corresponding regions of stability. Thus we arrive at a very important conclusion: the correlated hopping term can induce a insulator–metal transition, even in the half-filled-band case. Another important result, confirming the crucial role of the correlated hopping term, can be seen from figure 1, where a comprehensive phase diagram for the two-dimensional FKM with correlated hopping is presented. It is seen that the correlated hopping can destroy the CDW state, even at large values of the Coulomb interaction ($U \sim 7$). This is an unexpected result, since recent results of Wojtkiewicz and Lemanski [12] based on the combination of the perturbation expansion (up to second order) and the method of restricted phase diagrams predicted that the ground state of the model at $E_f = 0$ and U large is the CDW state for all values of $0 < t' < 1$. This discrepancy is probably due to the fact that the authors examined (as possible ground states) only a restricted set of configurations (consisting of all periodic configurations having elementary cells up to 12 sites), and the segregated configuration (which should be the ground state in this region) does not belong to this set. Another possible explanation of this discrepancy is that the second-order perturbation expansion used by the

[2] Since we consider the case $N_f + N_d = L$, the Fermi level E_F and the energy gap Δ of a configuration w are given by $E_F = \lambda_{L-N_f}$ and $\Delta = \lambda_{L-N_f+1} - \lambda_{L-N_f}$, respectively.

authors is insufficient to describe correctly the ground-state properties of the model in this region ($U \sim 7$).

The fact that the correlated hopping can induce metal–insulator transitions indicates that the picture of valence and metal–insulator transitions found in our previous papers within the conventional FKM [5,6,16] should be dramatically changed if finite values of t' are considered. The largest changes are expected in the strong-coupling limit ($U > 4$), where all ground states of the conventional FKM are insulating for both 1D and 2D case [5,13,16], while the numerical results obtained for non-zero t' indicate the existence of a metallic phase, at least for $n_f = 1/2$. We suppose that this important result is not restricted to the half-filled-band case only, but holds also for f-electron densities away from this point. To verify this conjecture, we have performed an exhaustive study of the model for $n_f = 1/4$ on 6×6, 8×8, and 12×12 clusters. Our numerical calculations showed that the phase diagram of the model at $n_f = 1/4$ is separated into two distinct regions. In the first region ($U < 2$) the phase diagram has a complex structure with the ground state apparently changing point by point at every value of the correlated hopping amplitude t' for fixed interaction strength. Unfortunately, the structure of the phase diagram in this region strongly depends on the size of the cluster and thus we were not able to extrapolate these results satisfactorily to the thermodynamic limit $L \to \infty$. In contrast to this case, the phase diagram exhibits a very simple structure (see the inset in figure 1) in the opposite limit ($U > 2$). In this region only two configurations are ground states of the FKM with correlated hopping—namely, the segregated configuration and the configuration w_4 (see figure 2) that has been proven to be the ground state of the conventional FKM for large U (see [16, 17]). Since the configuration w_s is metallic and w_4 insulating, we have correlated hopping-induced metal–insulator transitions also at $n_f = 1/4$. The metallic phase is stable up to $U \sim 7$ and this again confirms our conjecture that the comprehensive picture of metal–insulator transitions in the FKM with correlated hopping will be very different from the one found for the conventional FKM, especially for U large. To complete this picture, one has to perform similar calculations for all f-electron densities which is an onerous computational task, even for the 8×8 cluster. Work on this is currently in progress.

In summary, the effects of correlated hopping on the ground-state properties of the FKM in two dimensions have been studied. It was shown that the ground-state phase diagram as well as the picture of metal–insulator transitions found for the conventional FKM are substantially changed when the correlated hopping term is added. The effect of correlated hopping is so strong that it can induce a insulator–metal transition, even in the strong-coupling limit, where the ground states of the conventional FKM are insulating for all f-electron densities.

Acknowledgments

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.

References

[1] Falicov L M and Kimball J C 1969 *Phys. Rev. Lett.* **22** 997
[2] Freericks J K and Falicov L M 1990 *Phys. Rev.* B **41** 2163
[3] Gruber Ch, Lebowitz J L and Macris M 1993 *Phys. Rev.* B **48** 4312
[4] Ramirez K and Falicov L M 1971 *Phys. Rev.* B **3** 2455
[5] Farkašovský P 1995 *Phys. Rev.* B **51** 1507
[6] Farkašovský P 1995 *Phys. Rev.* B **52** R5463
[7] Farkašovský P 1996 *Phys. Rev.* B **54** 7856
[8] Farkašovský P 1997 *Phys. Rev.* B **54** 11 261

[9] Freericks J K and Zlatic V 1998 *Phys. Rev.* B **58** 322
See also Zlatić V, Freericks J K, Lemanski R and Czycholl G 2001 *Preprint* cond-mat/0107040
[10] Hubbard J 1963 *Proc. R. Soc.* A **276** 238
[11] Hirsch J E 1989 *Physica* C **158** 236
[12] Wojtkiewicz J and Lemanski R 2001 *Preprint* cond-mat/0106200
See also Michielsen K 1993 *Int. J. Mod. Phys.* B **7** 2571
[13] Lemberger P 1992 *J. Phys. A: Math. Gen.* **25** 715
[14] Farkašovský P and Gál S 2002 *Phase Transitions* at press
[15] Farkašovský P 1995 *J. Phys.: Condens. Matter* **7** 3001
Farkašovský P 1995 *J. Phys.: Condens. Matter* **7** 9775
[16] Farkašovský P 2001 *Eur. J. Phys.* B **20** 209
[17] Kennedy T 1994 *Rev. Math. Phys.* **6** 901