Phase transitions induced by correlated hopping in
the Falicov-Kimball model

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Abstract

The extrapolation of finite-cluster calculations is used to examine ground-
state properties of the one-dimensional Falicov-Kimball model with correlated
hopping. It is shown that the correlated hopping strongly influences both
the valence transitions and the conducting properties of the model and so it
should not be neglected in the correct description of materials with correlated
electrons. This is illustrated for two selected values of the Coulomb interaction
that represent typical behavior of the model for small and intermediate (strong)
interactions. In both cases the insulator-metal transitions (accompanied by
continuous or discontinuous valence transitions) induced by correlated hopping
are observed.

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1 Introduction

Recent theoretical studies of the Falicov-Kimball model (FKM) \[1\] showed that although this model is relatively simple, it can yield the correct physics for describing rare-earth and transition metal compounds \[2, 3\]. The model is based on the coexistence of two different types of electronic states in given materials: localized, highly correlated ionic-like states and extended, uncorrelated, Bloch-like states. The Hamiltonian of the model is given by sum of three terms

\[
H = \sum_{\langle ij \rangle} t_{ij} d_i^+ d_j + U \sum_i d_i^+ d_i f_i^+ f_i + E_f \sum_i f_i^+ f_i. \tag{1}
\]

The first term of (1) is the kinetic energy corresponding to quantum mechanical hopping of the itinerant \(d\) electrons between sites \(i\) and \(j\). Usually it is assumed that \(t_{ij} = -t\) if \(i\) and \(j\) are nearest neighbors and zero 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. The second term represents the Coulomb interaction between \(f\) electrons with density \(n_f = \frac{N_f}{L} = \frac{1}{L} \sum_i f_i^+ f_i\) and \(d\) electrons with density \(n_d = \frac{N_d}{L} = \frac{1}{L} \sum_i d_i^+ d_i\), where \(L\) is the number of lattice sites. The last term stands for the localized \(f\) electrons whose sharp energy level is \(E_f\).

One can see, that the interaction term in the conventional FKM includes only the local interactions and all nonlocal interactions are neglected. It is interesting to ask, however, if these nonlocal interactions are really unimportant and can be neglected or not. The possible improvement of the conventional FKM, which take into account also nonlocal interactions between nearest neighbors, is so-called correlated hopping term that describes how the occupancy of \(f\) orbitals influences the hopping probability of \(d\) electrons:

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

The importance of the correlated hopping term has already been mentioned by Hubbard \[4\]. Later Hirsch \[5\] pointed out that this term may be relevant in the explanation of superconducting properties of strongly correlated electrons. The effect of correlated hopping on the ground-state properties of the FKM has been examined recently by Gajek and Lemański in 1D \[6\] as well as Wojtkiewicz and Lemański in two dimensions \[7\]. The same subject has been studied in our previous papers \[8, 9\].
Using finite-cluster diagonalization calculations we have showed that the picture of valence and metal-insulator transitions is dramatically changed if the term of 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 $n_d = n_f = 1/2$ [9], where the ground state of the conventional FKM is insulating for all Coulomb interactions [10]. In the present paper we go beyond this case and examine a more general point $n_d + n_f = 1$, that is the point of the 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.

Since in the spinless version of the FKM (1) with correlated hopping (2) the $f$-electron occupation number $f_i^+ f_i$ of each site $i$ commutes with the Hamiltonian, 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 of the FKM with correlated hopping can be rewritten as

$$H = \sum_{(ij)} h_{ij}(w)d_i^+ d_j + E_f \sum_i w_i, \quad (3)$$

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

$$\tilde{t}_{ij}(w) = t_{ij} + t'_{ij}(w_i + w_j). \quad (4)$$

Thus for a given $f$-electron configuration $w = \{w_1, w_2, \ldots, w_L\}$ the Hamiltonian (3) is the second-quantized version of the single-particle Hamiltonian $h(w)$, so the investigation of the model (3) is reduced to the investigation of the spectrum of $h$ for different configurations of $f$ electrons. This can be performed exactly (over the full set of $f$-electron configurations) or approximatively (over the incomplete set, but still keeping the high precision of calculations). Here we adopt the second method since it allows us to treat several times larger lattices and so to minimize finite-size effects.
2 The method

The method used in this paper to study effects of correlated hopping on ground-state properties of the FKM is a simple modification of the finite-cluster exact-diagonalization method. This method was used firstly by one of us to describe the ground-state phase diagram (in $E_f - U$ plane) of the conventional FKM in one and two dimensions \[11\]. It was shown that the method is able to reproduce satisfactorily the exact results even after a relatively small number of iterations for both, one and two dimensions. The method is relatively simple and consists of the following steps: (i) Chose a trial configuration $w = \{w_1, w_2, \ldots, w_L\}$. (ii) Having $w, U, t'$ and $E_f$ fixed, find all eigenvalues $\lambda_k$ 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 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 given $U$ and $E_f$) is reached.

Of course, one can move instead of one electron (in step (iv)) two or more 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 $1 \leq p \leq p_{max}$ electrons ($p$ 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. Moreover, we have found that the method convergence depends sensitively on model parameters and selected values of $p_{max}$. Thus the first step in our numerical calculations was to find the optimum value of $p_{max}$ for the intermediate interactions, the case studied in this paper. In particular, we have tested the convergence of method for $U = 2$ and four selected values of $p_{max}$, and namely, $p_{max} = 1, 2, 3$ and $N_f$. The results of numerical calculations are summarized in Fig. 1, where the quantity $M_0$ (the minimal number of iterations for which the exact ground state for given $L$ is reached) is plotted as a function of $1/L$. It is seen, that selected $p_{max}$ strongly influence the method convergence, especially for large $L$, where the cases $p_{max} = 1$ and $p_{max} = N_f$ need several
times larger number of iterations than the cases \( p_{\text{max}} = 2 \) and \( p_{\text{max}} = 3 \). Therefore, we chose the case \( p_{\text{max}} = 2 \) for the numerical calculations in the intermediate region.

3 Results and discussion

The main aim of this paper is to answer the question, how the correlated hopping influences ground-state properties of the one-dimensional FKM in the symmetric case (\( E_f = 0, n_f + n_d = 1 \)). In particular, the influence of \( t' \) on valence transitions and conducting properties of the model was studied. We present results for two selected values of the Coulomb repulsion interaction, namely \( U = 1 \) and \( U = 2 \). The value \( U = 1 \) represents the typical behavior of the system for weak interactions and the value \( U = 2 \) represents the behavior of the system for intermediate and strong interactions. The ground states were studied exactly on the finite clusters consisting of \( L = 12, 16, 20 \) and \( 24 \) lattice sites, while for larger lattices (up to \( L = 120 \)) the approximate method, discussed above, was used. It is well-known, that the \( f \)-electron density \( (n_f) \) for the symmetric FKM without correlated hopping is equal to \( 1/2 \) and the system is an insulator for all \( U > 0 \) \([10]\). It is interesting to ask, if the non-zero correlated hopping can change this picture.

\textbf{U = 1}

To examine the influence of correlated hopping on the valence transition we have performed an exhaustive study of the model on finite clusters (up to \( L = 60 \)) for \( t' \) ranging from \(-2 \) to \( 2 \) with step \( 0.02 \). Results of numerical calculations are displayed in Fig. 2 for three selected clusters (\( L = 24, 48 \) and \( 60 \)) and they clearly demonstrate the strong effects of correlated hopping on the valence transitions. For each of these lattices \( n_f \) exhibits the same characteristic features: (i) On the interval \([ -0.38, 0.4 ]\) the \( f \)-electron concentration is equal to \( 0.5 \) (like for the conventional FKM). (ii) Below \( t' = -0.38 \) the \( f \)-electron occupation number increases. (iii) Above \( t' = 0.4 \) the \( f \)-electron density rapidly falls down from \( n_f = 0.5 \) to \( n_{f\text{min}} \sim 0.25 \) and then gradually increases. Due to the fact that we have considered finite (although relatively large) lattices the valence transitions have a stair-case structure, which is gradually suppressed with increasing \( L \), of course with the exception of the stair at \( t' = 0.4 \)
that seems to be independent of $L$. A detailed analysis showed (see Fig. 2d) that the valence transition from $n_f = 1/2$ to $n_{f\text{min}} \sim 1/4$ is not discontinuous, but it is realized through the consecutive intermediate-valence transitions (on the interval $[0.4, 0.44]$) followed by continuous changes of $n_f (L \to \infty)$ for $t' > 0.44$. The similar behavior was observed also for negative $t' (t' < -0.38)$.

Moreover, our numerical results showed that there are three critical values of $t'$ where $n_f$ changes its character. For negative values of correlated hopping $t'_{c1} \sim -0.38$ was observed. For $t' > 0$ two critical values of correlated hopping $t'_{c2} \sim 0.4$ and $t'_{c3} \sim 0.54$ were found. The numerical results showed that the ground state between $t'_{c1}$ and $t'_{c2}$ is the alternating configuration. For $t' > t'_{c3}$ the ground states are the segregated configurations with different $N_f$. Between $t'_{c2}$ and $t'_{c3}$ a few configuration types are stable:

(i) The most homogeneous configurations with $N_f < L/2$.

(ii) The mixtures of the alternating configuration $(w_a)$ and the empty configuration $(w_0)$.

(iii) The mixtures of the empty configuration $(w_0)$ and some periodic configurations $(w_p)$ (e.g. $w_{(L=20)} = \{11101100000000000000\}$).

(iv) Around the boundary of two configuration types $w_A, w_B$ mixtures $w_A \& w_B$ are observed.

The ground-state configurations for $t' < t'_{c1}$ but near $t'_{c1}$ are the most homogeneous configurations with $N_f > L/2$ and for smaller values of $t'$ there are the mixtures of the alternating configuration $(w_a)$ and the fully occupied configuration $(w_1)$. Lastly, mixtures of periodic configurations and the alternating configuration $(w_p \& w_a)$ are observed.

Since the ground states of the FKM with correlated hopping consist of configurations which are different from the alternating configuration (that is the ground state for the conventional FKM) it is natural to expect that the correlated hopping will change also the conducting properties of the model. To verify this conjecture the energy gap ($\Delta = \lambda_{L-N_f+1} - \lambda_{L-N_f}$) at the Fermi level was calculated for different finite clusters. Fig. 3 shows the energy gap on the interval $t' = [-2, 2]$ for
two clusters of \( L = 36 \) and 48 sites at \( U = 1 \). In the region where the alternating phase is the ground state the gap \( \Delta \) has a finite value \((\Delta = U)\) independent of \( L \), and so the system is an insulator. This conclusion is identical with the conventional FKM \((t' = 0)\). At \( t' \sim 0.4 \) the energy gap changes from \( \Delta = U \) to \( \Delta \sim U/2 \) for both examined lattices (the inset in Fig. 3). The detailed analysis showed that the most homogeneous configurations are the ground states for \( t' \) between \( t' \sim 0.4 \) and \( t' \sim 0.44 \) where \( \Delta \sim U/2 \). The extrapolation of the finite-cluster results to the thermodynamic limit at \( t' = 0.42 \) confirmed, that the energy gap has a finite value for \( L \to \infty \) and the system is really an insulator in this region (Fig. 4). On Fig. 4 we plotted also extrapolated results for three other positive values of \( t' \) \((t' = 0.5, 0.55 \) and \( 2 \)). Their fits obviously converge to zero (the metallic state) indicating that the correlated hopping induces the insulator-metal transition at \( t' \sim 0.44 \). To find the complete picture of metal-insulator transitions in the FKM with correlated hopping we have performed also an exhaustive study of the model for a wide region of negative values of \( t' \) \((t' \in [-2, -0.38])\). A similar behavior of the model has been observed. For \( t' \) between \( t' \sim -0.5 \) and \( t' \sim -0.38 \), where the ground states are the most homogeneous configurations, the energy gap has a finite value \( \Delta \sim U/2 \), while for \( t' \) between \( t' \sim -1 \) and \( t' \sim -0.5 \) the energy gap vanishes in the thermodynamic limit. This is illustrated in Fig. 5, where the energy gap \( \Delta \) is plotted for several values of \( t' \) as a function of \( 1/L \). The comprehensive picture of insulator-metal transitions in the thermodynamic limit obtained from extrapolated behaviors is displayed in Fig. 6 and clearly demonstrates that the correlated hopping dramatically changes the conducting properties of the model. In addition to an insulating phase, which characterizes the conventional FKM, the large metallic phases are found for the FKM with correlated hopping. The metallic phases are observed for positive and also for negative \( t' \). For \( t' > 0 \) there exists the wide metallic region above \( t' \sim 0.44 \) and for \( t' < 0 \) there exists the wide metallic region, between \( t' \sim -1 \) and \( t' \sim -0.5 \). For positive as well as negative \( t' \) the transition from the insulating to metallic phase realizes through two discontinuous transitions. The first is the insulator-insulator transition from \( \Delta = U \) to \( \Delta \sim U/2 \) and the second is the insulator-metal transition from \( \Delta \sim U/2 \) to \( \Delta = 0 \). Unfortunately, we were not able to determine the type of transition (continuous or discontinuous) at \( t' \sim -1 \). The finite-size effects near this transition point are still
large, and so it was very difficult to do definite conclusions concerning the transition type. Our results only indicate that the transition at $t' \sim -1$ is probably continuous.

$U = 2$

The same procedure as for $U = 1$ has been used also for $U = 2$. As was mentioned above this value represents the typical behavior of the system for intermediate and strong interactions. Again we have performed a study of the model on finite clusters (up to $L = 60$) for $t'$ running from $-2$ to $2$ with step $0.02$. Fig. 7a shows the valence transition for the cluster with $L = 48$ sites, which qualitatively describes $n_f$ for this interaction case. It is seen, that the valence transition has a similar character as for $U = 1$. In particular, there exists the region (between $t'_{c_1} \sim -0.78$ and $t'_{c_2} \sim 0.66$), where the $f$-occupation number is constant and equal to $1/2$. Below $t'_{c_1}$ the $f$-electron occupation number increases from $n_f = 0.5$, and above $t'_{c_2}$ the $f$-electron density rapidly falls down from $n_f = 0.5$ to $n_{f_{\text{min}}} \sim 0.42$ and then gradually increases, similarly as for $U = 1$. However, there is one important difference. The detailed analysis performed on finite clusters up to $L = 60$ showed, that the valence transition at $t'_{c_2}$ changes discontinuously from $n_f = 0.5$ to $n_{f_{\text{min}}} \sim 0.42$. Moreover, comparing the valence transitions for $U = 1$ and $U = 2$ one can see, that the stronger Coulomb interaction needs the larger $t'$ (in the absolute value) to change the ground state from $n_f = 1/2$ to another $n_f$.

Also for this case, we have tried to describe the ground-state configurations. Although the phase diagram is very complex we were able to describe the basic configuration types. Between $t'_{c_1}$ and $t'_{c_2}$ the alternating configuration is the ground state for all investigated lattices. For $t' > t'_{c_2}$ the ground states are the segregated configurations with different $N_f$. Below $t'_{c_1}$ we were able to specify several configuration types with the significant stability regions. In particular:

(i) The most homogeneous configurations with different $N_f > L/2$.

(ii) The mixtures of the alternating configuration ($w_a$) and the fully occupied configurations ($w_1$) of different length.
(iii) The mixtures of the alternating configuration \( (w_a) \) and periodic configurations \( (w_p) \).

To calculate the energy gap for \( U = 2 \) the same procedure, the extrapolation of finite-cluster calculations (up to \( L = 120 \)), was used. The extrapolated values of the energy gap are plotted in Fig. 7b as a function of \( t' \). Comparing the energy gaps for \( U = 1 \) and \( U = 2 \) (Fig. 6 and Fig. 7b), one can see that they exhibit qualitatively same behaviors. In particular, there is the wide insulating region around \( t' = 0 \), two wide metallic regions (one for positive and one for negative \( t' \)) and the insulating region below the metallic one for negative \( t' \). On the other hand, the careful analysis showed one important difference between the case \( U = 1 \) and \( U = 2 \). Namely, for \( U = 2 \) and \( t' > 0 \) the system undergoes discontinuous insulator-metal transition from \( \Delta = U \) to \( \Delta = 0 \), while for \( U = 1 \) the system undergoes two discontinuous transitions (the insulator-insulator transition from \( \Delta = U \) to \( \Delta \sim U/2 \) and the insulator-metal transition from \( \Delta \sim U/2 \) to \( \Delta = 0 \)). Moreover, one can see that with increasing \( U \) the metallic regions shift to larger values (in the absolute value) of correlated hopping.

Thus we can conclude that the correlated hopping \( t' \) plays the crucial role in description of the ground-state properties of the spinless FKM in 1D. The non-zero values of \( t' \) substantially change the valence transitions as well as the conducting properties of the model (in comparison with the conventional FKM). For the valence transitions it was found that the relatively small values of \( t' \) can induce the large changes of \( n_f \) and these changes can be continuous as well as discontinuous. However, the most important result is that the correlated hopping can induce the insulator-metal transitions in the FKM for both positive and negative values of \( t' \). These results clearly show that the correlated hopping strongly influences the ground-state properties of the FKM and so it should not be neglected in the correct description of real materials with correlated electrons. Of course, to do a direct comparison with experimental measurements one has to study FKM with correlated hopping in large dimensions. Work on this subject is currently in progress.

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Figure 1: Dependence of the iteration number $M_0$ on $1/L$ for the intermediate Coulomb interaction $U = 2$ and four different values of $p_{max}$. 
Figure 2: Dependence of the valence transition on the correlated hopping $t'$ for different finite clusters at $U = 1$. For $L = 24$ (a), $L = 48$ (b) and $L = 60$ (c) calculations have been done with step 0.02 and $M = 2000$. Results for $L = 480$ and 960 (d) have been obtained on the extrapolated set of ground-state configurations in this region (the most homogeneous configurations and the mixtures of the alternating and empty configurations).
Figure 3: Dependence of the energy gap $\Delta$ on the correlated hopping $t'$ (calculated with step 0.02) for two finite clusters of $L = 36$ and $L = 48$ sites ($U = 1$, $M = 2000$). The inset shows the energy gap for the same clusters on the interval $[0.35, 0.5]$ calculated with step 0.002 and $M = 10000$. 
Figure 4: The polynomial fits of energy gaps for $U = 1$ and four positive values of $t'$. 

\[ E = \frac{1}{L} \]
Figure 5: The polynomial fits of energy gaps for $U = 1$ and four negative values of $t'$. 
Figure 6: Dependence of the energy gap $\Delta$ on the correlated hopping $t'$ for $L \to \infty$ and $U = 1$, calculated from extrapolated behaviors. The data between $t' \sim -0.5$ and $t' \sim 0.44$ were obtained on the extrapolated set of ground-state configurations (the most homogeneous configurations).
Figure 7: (a) Dependence of the valence transition on the correlated hopping $t'$ for the finite cluster of $L = 48$ sites and $U = 2$, calculated with $M = 2000$ iterations. (b) Dependence of the energy gap $\Delta$ on the correlated hopping $t'$ for $L \to \infty$ and $U = 2$, obtained from extrapolated behaviors. The data between $t' \sim -1$ and $t' \sim -0.78$ were extrapolated from the most homogeneous configurations.