The influence of hopping on valence transitions in the Falicov-Kimball model

1995 J. Phys.: Condens. Matter 7 3001

(http://iopscience.iop.org/0953-8984/7/15/007)

J. Phys.: Condens. Matter 7 (1995) 3001–3012. Printed in the UK

The influence of hopping on valence transitions in the Falicov–Kimball model

Pavol Farkašovský

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

Received 8 December 1994, in final form 25 January 1995

Abstract. We use strong-coupling perturbation theory and the extrapolation of small-cluster exact-diagonalization calculations to describe the ground-state properties and possible intermediate-valence transitions of the spinless Falicov–Kimball model with a generalized type of hopping. It is shown that, even for relatively small values of the interaction strength, the Falicov–Kimball model undergoes only a few (discrete) intermediate-valence transitions, and this result is demonstrated to be independent of finite-size effects.

1. Introduction

Since its introduction in 1969, the Falicov–Kimball model [1] has become an important standard model for a description of correlated fermions on a lattice. The model describes a two-band system of localized f electrons and itinerant d electrons with a short-range f–d Coulomb interaction U. The Hamiltonian is

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

where f_i^+, f_i are the creation and annihilation operators for an electron in a 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; however, in what follows we consider a much more realistic type of hopping, so for the moment we leave it to be arbitrary.

Although the model has various physical interpretations (as well as the aforementioned interpretation it can be considered as a model for crystallization in a system of classical ions interacting with itinerant electrons [2], or as an approximation to the Hubbard model [3] in which only one kind of electron can hop), there exist two fundamental questions that have attracted the attention of physicists. The first is the nature of the ground state of the model and its energetic and structural properties. The second is the problem of metal–insulator and valence transitions in the spinless Falicov–Kimball model. In spite of its relative simplicity, so far only a few rigorous results concerning the ground state of the Hamiltonian (1) have been obtained: Brandt and Schmidt [4] found sharp upper and lower bounds for the ground-state energy in two dimensions; Kennedy and Lieb [2] proved that the ground state has long-range order for all dimensions d; Brandt and Mielsch [5] obtained

0953-8984/95/153001+12$19.50

an exact solution in $d = \infty$; Gruber [6] and Lyzwa [7] derived some rigorous results for a particular class of periodic configurations; Lemberger [8] proved two exact theorems in the limit of strong interactions; Gruber and co-workers [9] obtained a set of exact results pertaining to the neutral case, showing that the system forms atoms at sufficiently large U.

The second question, namely whether the Falicov–Kimball model can describe the discontinuous transition of the f-electron occupation number n_f as a function of the f-level energy E_f, is crucial for an understanding of some anomalous physical properties of rare-earth compounds. For example, supposing that the external pressure shifts the energy level E_f, then the valence transitions observed in some rare-earth compounds (SmS, TmTe, and so on) could be understandable purely electronically if $n_f(E)$ really has discontinuities. However, whether discontinuous valence transitions appear for the Falicov–Kimball model is again very sensitive to the approximations used.

Depending on the type of approximation used, both positive answers [1, 10–12] and negative answers [13–15] were found. Discontinuous transitions were obtained within Hartree–Fock treatments if the intra-atomic interaction term was decoupled in a form that was diagonal in the f and d creation and annihilation operators, while in much more reliable treatments based on the coherent-potential approximation no sign of any discontinuity was obtained. Thus, within the Hartree–Fock treatments, the Falicov–Kimball model can describe the first-order transition from $n_f = 1$ to $n_f = 0$; however the valence, i.e. the number of localized f electrons n_f, remains an integer and does not attain intermediate values. Although this shortcoming can be removed by including the hybridization of localized states with the band states, the theoretical picture of the transitions is still uncertain, since different approximations again produce controversial results [16–22]. From this short survey it is clear that the study of valence and metal–insulator transitions may be successful only with methods that are relatively insensitive to the type of approximation used and, of course, with the exact methods.

Exact results concerning this question are rare. The numerical calculations of Brandt and Schmidt [4] based on Tchebycheff–Markov inequalities show ($d = 2$) that for $E < E_1$ the ground state of the model is the fully occupied lattice ($n_f = 1, n_d = 0$). For $E_2 < E < E_3$ the ground state is a chessboard configuration ($n_f = 1/2, n_d = 1/2$) and for $E > E_4$ the ground state is the empty lattice ($n_f = 0, n_d = 1$). Unfortunately, the authors are unable to decide whether or not the valence transitions from $n_f = 1$ to $n_f = 1/2$ and from $n_f = 1/2$ to $n_f = 0$ are discontinuous.

To resolve this problem, in a previous paper [23] we used strong-coupling perturbation theory and the extrapolation of small-cluster exact-diagonalization calculations. We found that in the general case the transitions have a staircase structure. With increasing U this structure is maximally simplified, and only a few transitions become relevant. For $5 < U < 10$ there are only four relevant transitions: from $n_f = 1$ to $n_f = 2/3$, from $n_f = 2/3$ to $n_f = 1/2$, from $n_f = 1/2$ to $n_f = 1/3$ and from $n_f = 1/3$ to $n_f = 0$. For $U > 10$ there are only two relevant transitions: from $n_f = 1$ to $n_f = 1/2$ and from $n_f = 1/2$ to $n_f = 0$.

In the present paper the same methods are used for an investigation of the band effects (the type of hopping) on the valence transitions and ground-state properties of the model.

To study this subject we choose a more general form for the hopping matrix elements, namely

$$t_{ij} = -tq^{(L/2)-|i-j|-(L/2)|-1}(1-\delta_{ij}) \tag{2}$$

where L denotes the number of lattice sites and $q \leqslant 1$.

There are several advantages of this form. It represents a much more realistic type of hopping electrons on a lattice, and it allows us to change continuously the type of hopping (band) from nearest-neighbour ($q = 0$) to infinite-range ($q = 1$) [24] hopping and thus immediately study the effect of the conduction band on the physical properties of the model, particularly on the ground-state configuration and on the valence transitions, which have been the subject of much controversy [21].

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.

Thus the Hamiltonian (1) can be written as

$$H = \sum_{i,j} h_{ij} d_i^+ d_j + E_f \sum_i w_i \tag{3}$$

where $h_{ij}(w) = t_{ij} + U w_i \delta_{ij}$ and t_{ij} are given by (2). The investigation of (3) is now reduced to the investigation of the spectrum of h for different f-electron configurations.

2. Perturbative analysis

A previous paper [25] devoted to the investigation of the ground-state properties of the Falicov–Kimball model ($q = 0$) showed that the strong-coupling perturbation theory of degenerate levels is capable of closely reproducing the exact results of Freericks and Falicov [26] (obtained for the particular class of periodic configurations), even for relatively small values of the interaction strength, $U/t > 5$. Therefore, to reveal a qualitative picture of the valence transitions, we start with the strong-coupling limit of (3) and with perturbation theory of degenerate levels.

We can see that for a given f-electron configuration $w = \{w_1, w_2 \dots w_L\}$, defined on a one-dimensional lattice of L sites with periodic boundary conditions, the first term of (3) is the second-quantized version of the single-particle Hamiltonian $h = T + UW$, where T is the L-square matrix with elements t_{ij} given by (2) and W is the L-square diagonal matrix with elements w_i ($\sum_i w_i = N_f$ is the number of f electrons). Since the matrix W is idempotent, the matrix UW has only two eigenvalues $E_1 = 0$ and $E_2 = U$, which are $(L - N_f)$-fold and N_f-fold degenerate. Considering now the interaction energy UW of the Hamiltonian (3) as the unperturbed Hamiltonian and the kinetic energy as the perturbation, then the second-order corrections can be found directly using the standard perturbation theory of degenerate levels [23, 25]. For $E_1 = 0$ and $E_2 = U$ its application leads to the following secular equation:

$$\det(T^{(\pm)} - \lambda I) = 0. \tag{4}$$

Here $T^{(-)}$ and $T^{(+)}$ are $(L - N_f)$ and N_f square matrices with elements

$$T_{nn'}^{(\pm)} = t_{nn'} \pm \frac{1}{U} \sum_j t_{nj} t_{jn'} w_j \tag{5}$$

where n and n' denote unoccupied (occupied) sites if the second-order corrections to the energy level $E_1 = 0$ ($E_2 = U$) are calculated.

However using the theorem of Gersgorin [27], one can find that the electron spectra arising from the degenerate energy levels $E_1 = 0$ and $E_2 = U$ form, for $U > U_0 = 4/[(1-q^2)U]$, two non-overlapping bands with exactly $(L-N_f)$ and N_f states and thus the energy of $N_d = L-N_f$ electrons at the half-filled band point $N_f+N_d = L$ (next we consider only this case, which is the point of special interest for mixed-valence phenomena) can be obtained directly by occupying all $(L-N_f)$ energy levels λ_k corresponding to $E_1 = 0$, or in other words by taking the trace of $T^{(-)}$:

$$E(w, N_d = L - N_f) = \sum_{k=1}^{L-N_f} \lambda_k = \mathrm{Tr}(T^{(-)}) = \sum_i T_{ii}^{(-)}(1-w_i). \tag{6}$$

Now using (5), the total energy corresponding to any configuration $w = \{w_1, w_2 \ldots w_L\}$ with total f-electron number N_f can be written as

$$E(w, N_f) = -\frac{1}{U}\sum_{ij} t_{ij}t_{ji}(1-w_i)w_j + EN_f. \tag{7}$$

A straightforward analysis of (7) shows that, just as for $q = 0$ [8], for $q > 0$ the most homogeneous configurations are the ground states of the Falicov–Kimball model for sufficiently large U. This is obviously a consequence of the chosen form of the hopping matrix elements, which as one can immediately check for $N_f = 2, 3 \ldots$ forces the f electrons to be as separated as possible. Using this result we can directly study the valence transitions in the spinless Falicov–Kimball model at large U. However, before doing this, let us first investigate the model for small lattices to show that the most homogeneous configurations play a central role in valence transitions, not only for large U but also for relatively small values of U.

3. Numerical calculations

With regard to the aforementioned sensitivity of the valence and metal–insulator transitions to the type of approximation employed, we used for their description the extrapolation of small-cluster exact-diagonalization calculations. Since the d electrons do not interact among themselves, the numerical calculations proceed directly in the following steps. (i) Having U, E_f, q and $w = \{w_1, w_2 \ldots w_L\}$ fixed, find all eigenvalues λ_k of $h(w) = T + UW$. (ii) For a given $N_f = \sum_i w_i$ determine the ground-state energy $E(w, U, E_f) = \sum_{k=1}^{L-N_f} \lambda_k + E_f N_f$ of a particular f-electron configuration w by filling in the lowest $N_d = L - N_f$ one-electron levels. (iii) Find the w^0 for which $E(w, U, E_f)$ has a minimum.

Repeating this procedure for different values of U or E_f, one can immediately study the dependence of the f-electron occupation number $N_f = \sum_i w_i^0$ on U, E_f or q.

To demonstrate the influence of electron hopping on the valence transitions we start with the simplest case: $U = 0$. The numerical results obtained for finite systems are shown in figures 1 and 2. In figure 1 the E_f-dependence of the f-electron occupation density n_f is plotted for $L = 512$ sites and different values of q, whereas figure 2 illustrates the finite-size effect on the beginning (end) of transitions. The results show that (i) with q going from 0 to 1 the transition becomes much steeper, and even for the infinite-range hopping ($q = 1$) it is discontinuous, in agreement with analytical results [24]; (ii) only a behaviour with $q = 0$ (reflecting the particle–hole symmetry of the model) is point-symmetrical around $n_f(E_f = 0) = 0.5$; (iii) the beginning (end) of the transition is almost independent of L.

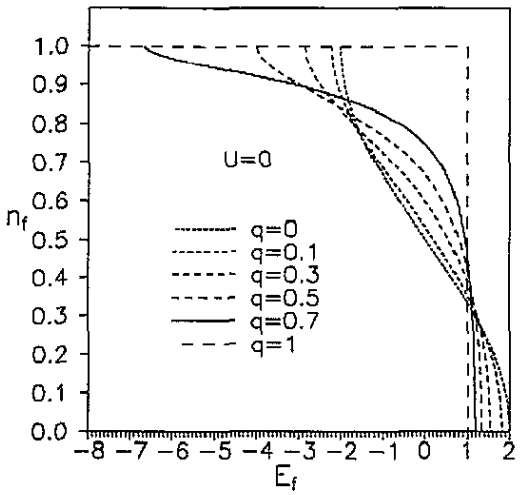

Figure 1. The dependence of the f-electron occupation number n_f on the f-level position E_f calculated for $L = 512$, $U = 0$ and six different values of q.

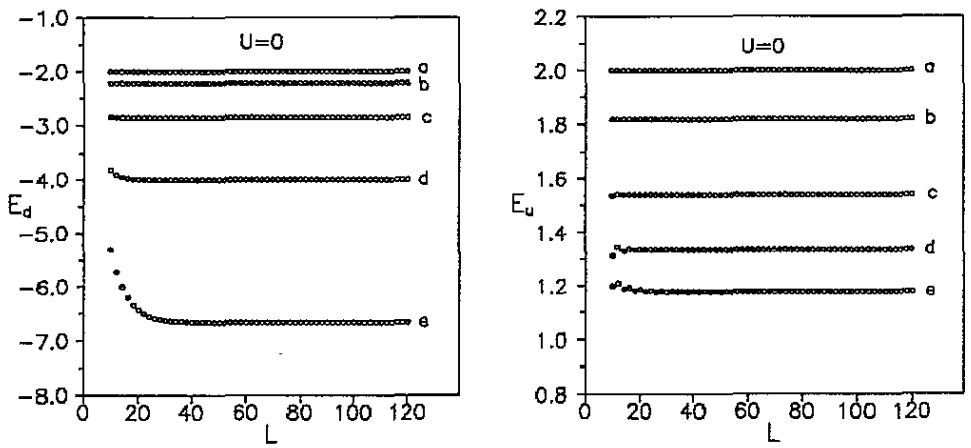

Figure 2. The L-dependence of the exact numerical bounds of the fully occupied (E_d) and completely empty (E_u) lattice calculated for $U = 0$ and (*a*) $q = 0$, (*b*) $q = 0.1$, (*c*) $q = 0.3$, (*d*) $q = 0.5$ and (*e*) $q = 0.7$.

The last observation is very important for the extrapolation of small-cluster exact-diagonalization calculations, since it indicates that at least some characteristics of the transitions are independent of L. However, from a theoretical point of view, the first observation showing the possibility of discontinuous valence transitions is also very interesting.

Let us now incorporate many-body effects and study the model for non-zero U. The results obtained for small finite systems of $L = 12$ and 20 sites, and for the set of the interaction strengths $U = 1.5, 3, 4.5$, are presented in tables 1 and 2 and in figures 3 and 4 (here and in what follows all energies are measured in units of t).

We summarize these results with some observations. (i) For $q = 0.1$ and the given set of

Table 1. Ground-state configurations for $L = 12$, $U = 3$ and $q = 0.1, 0.3, 0.5, 0.7$.

N_f	$q = 0.1$	$q = 0.3$	$q = 0.5$	$q = 0.7$
0	000 000 000 000	000 000 000 000	000 000 000 000	000 000 000 000
1	100 000 000 000	100 000 000 000	100 000 000 000	100 000 000 000
2	100 000 100 000	101 000 000 000	101 000 000 000	100 100 000 000
3	100 010 001 000	101 010 000 000	101 010 000 000	100 010 001 000
4	100 100 100 100	101 010 100 000	101 010 100 000	100 100 100 100
5	100 101 001 010	101 010 101 000	101 010 101 000	100 101 010 010
6	101 010 101 010	101 010 101 010	101 010 101 010	101 010 101 010
7	101 011 010 110	110 101 011 010	110 110 101 010	110 110 101 010
8	110 110 110 110	110 110 110 110	110 110 110 110	110 110 110 110
9	111 011 101 110	111 011 101 110	111 011 101 110	111 011 101 110
10	111 110 111 110	111 110 111 110	111 110 111 110	111 110 111 110
11	111 111 111 110	111 111 111 110	111 111 111 110	111 111 111 110
12	111 111 111 111	111 111 111 111	111 111 111 111	111 111 111 111

Table 2. Ground-state configurations for $L = 20$, $U = 3$ and $q = 0.3, 0.7$.

N_f	$q = 0.3$	$q = 0.7$
0	00 000 000 000 000 000 000	00 000 000 000 000 000 000
1	10 000 000 000 000 000 000	10 000 000 000 000 000 000
2	10 100 000 000 000 000 000	10 010 000 000 000 000 000
3	10 101 000 000 000 000 000	10 010 010 000 000 000 000
4	10 101 010 000 000 000 000	10 010 010 010 000 000 000
5	10 101 010 100 000 000 000	10 010 010 010 010 000 000
6	10 101 010 101 000 000 000	10 010 010 010 010 010 000
7	10 101 010 101 010 000 000	10 010 100 100 100 100 100
8	10 101 010 101 010 100 000	10 010 101 010 100 100 100
9	10 101 010 101 010 101 000	10 010 101 010 101 010 100
10	10 101 010 101 010 101 010	10 101 010 101 010 101 010
11	11 010 101 010 110 101 010	11 011 010 101 010 101 010
12	11 010 110 101 101 011 010	11 011 011 010 101 010 110
13	*11 011 011 011 011 011 010*	*11 011 011 011 011 011 010*
14	11 101 101 101 110 110 110	11 101 110 110 110 110 110
15	11 101 110 111 011 101 110	11 101 110 111 011 101 110
16	11 110 111 101 111 011 110	11 110 111 101 111 011 110
17	11 111 101 111 110 111 110	11 111 011 111 101 111 110
18	11 111 111 101 111 111 110	11 111 111 101 111 111 110
19	11 111 111 111 111 111 110	11 111 111 111 111 111 110
20	11 111 111 111 111 111 111	11 111 111 111 111 111 111

U, the ground-state configurations of the Falicov–Kimball model are the most homogeneous configurations. This means that the most homogeneous distribution of the f electrons, first found by Lemberger [8], for $q = 0$ and sufficiently large U persists for small but non-zero values of q. (ii) For larger values of q the mixture of two crenel configurations $[p|m]$ may be the ground state. (The unit cell of the crenel configuration $[p|m]$ consists of p consecutive sites occupied by the f electrons, while $m - p$ sites are empty.) Whereas for $n_f < 1/2$ the mixtures of the crenel configurations $[1|m]$ with $m = 2, 3 \ldots$ and the empty configuration appear most often, for $n_f > 1/2$ it is the mixture of $[p|p + 1]$ and $[p - 1|p]$ crenel configurations. (iii) The alternating phase $\{1010 \ldots\}$ is the ground state at $n_f = 1/2$ for all values of U and q. The very existence of this intermediate-valence state with a chessboard structure is an important characteristic of the valence transitions, since it appears for each transition and the region of its stability is almost independent of

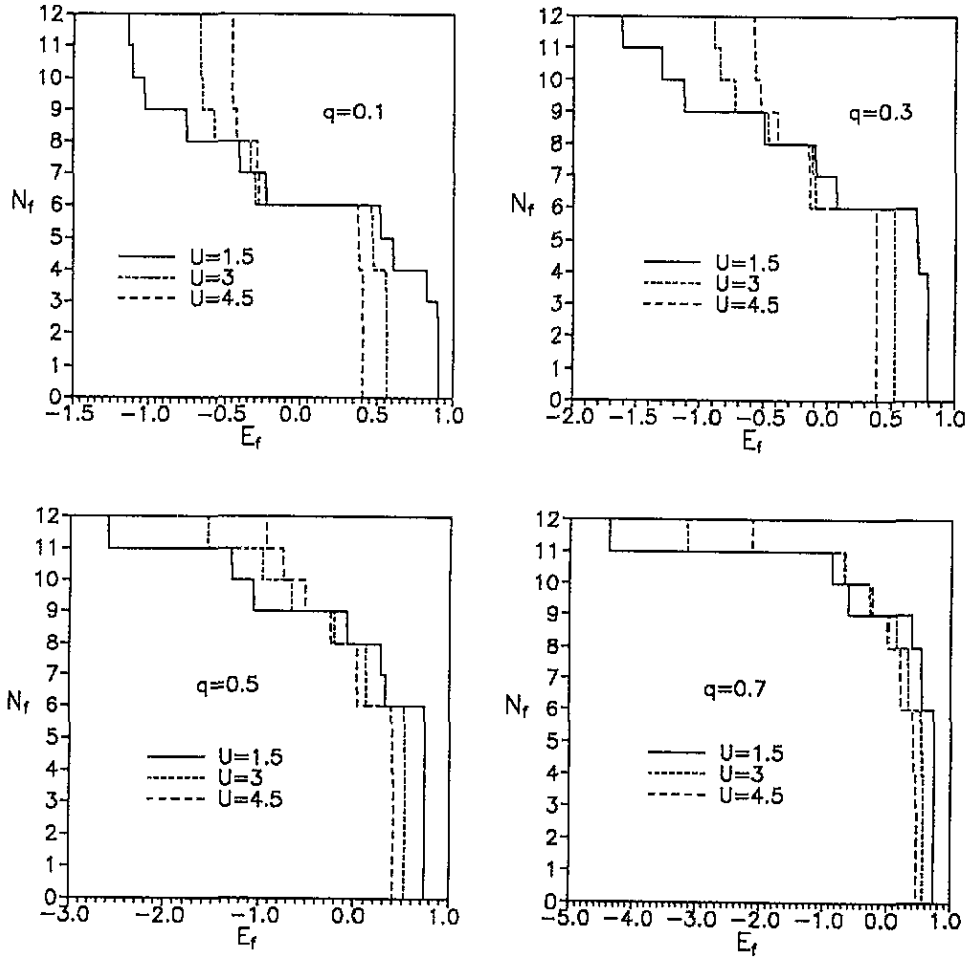

Figure 3. The dependence of the f-electron occupation number N_f (calculated for all configurations) on the f-level position E_f for $L = 12$, $U = 1.5, 3, 4.5$, and $q = 0.1, 0.3, 0.5, 0.7$.

L. As follows from the preceding figures, the same is true for the beginning (end) of the transitions. (We will discuss more accurate finite-size effects on these quantities below). (iv) The valence transitions have, in general, a staircase structure, which strongly depends on U and q. However, with increasing U and q this structure is maximally simplified and for sufficiently large U or q only a few transitions become relevant. For example, while for $q = 0.1$ and the given set of U there are several transitions from $n_f = 1/2$ to $n_f = 0$, for $q = 0.5$ there is only one relevant transition independent of L and U. Furthermore, with increasing q the transitions are much steeper, the region of stability of the intermediate-valence state with chessboard structure being gradually suppressed, and unlike the case of small values of q a direct transition from $n_f = 0$ to $n_f > 1/2$ is possible for $q > 0.9$. (v) There exist several characteristics of the valence transitions that are independent, or almost independent, of L. As well as the characteristics mentioned above, i.e. the beginning (end) of the transition, the region of stability of the intermediate-valence state with chessboard structure is also the length of stairs corresponding to configurations with $n_f = 1 - 1/i$ ($E < 0$) or $n_f = 1/i$ ($E > 0$), $i = 1, 2 \ldots L$.

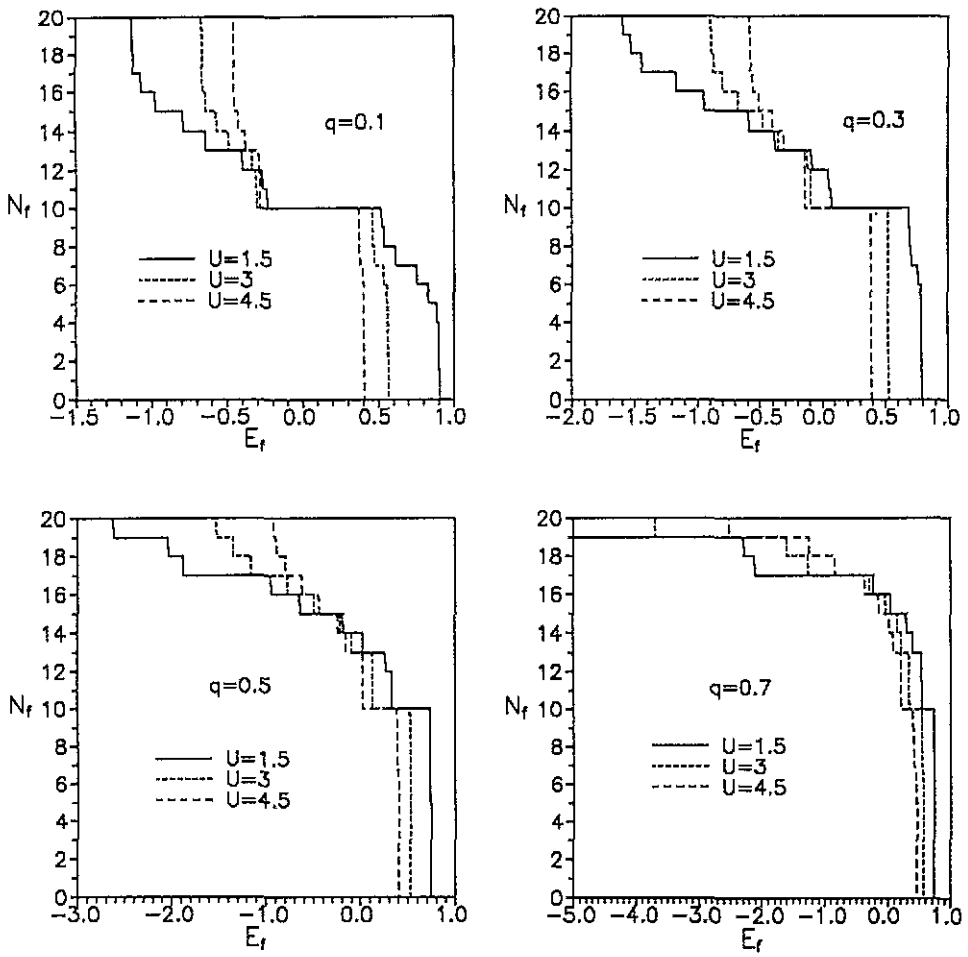

Figure 4. The dependence of the f-electron occupation number N_f (calculated for all configurations) on the f-level position E_f for $L = 20$, $U = 1.5, 3, 4.5$ and $q = 0.1, 0.3, 0.5, 0.7$.

To determine the finite-size effects more accurately, the L-dependence of the exact numerical bounds for the most interesting ground states, i.e. when (i) the lattice is completely filled with f electrons (yielding the value of the beginning of the valence transitions, E_d), (ii) it is completely empty (the end of the transition, E_u) and (iii) it has a chessboard structure (E_{a_1}, E_{a_2}), have been calculated. The results presented in figure 5 show that only for $q \to 1$ can a weak dependence of bounds on L be observed. This indicates that at least some characteristics of the valence transitions in the thermodynamic limit may be deduced from characteristics of the valence transitions of finite systems. However, for further investigation of the valence transitions the most important fact was that the valence transitions calculated only for the most homogeneous configurations are practically identical with these shown in figures 3 and 4. Negligible differences may be observed only if the calculations are done with a step $\Delta E_f \leqslant 0.005$. This fact indicates that the basic structure of the valence transitions can be described very precisely taking into account only the most homogeneous configurations, and at the same time it allows us to avoid technical difficulties associated with a large number of configurations and consequently to study much larger systems.

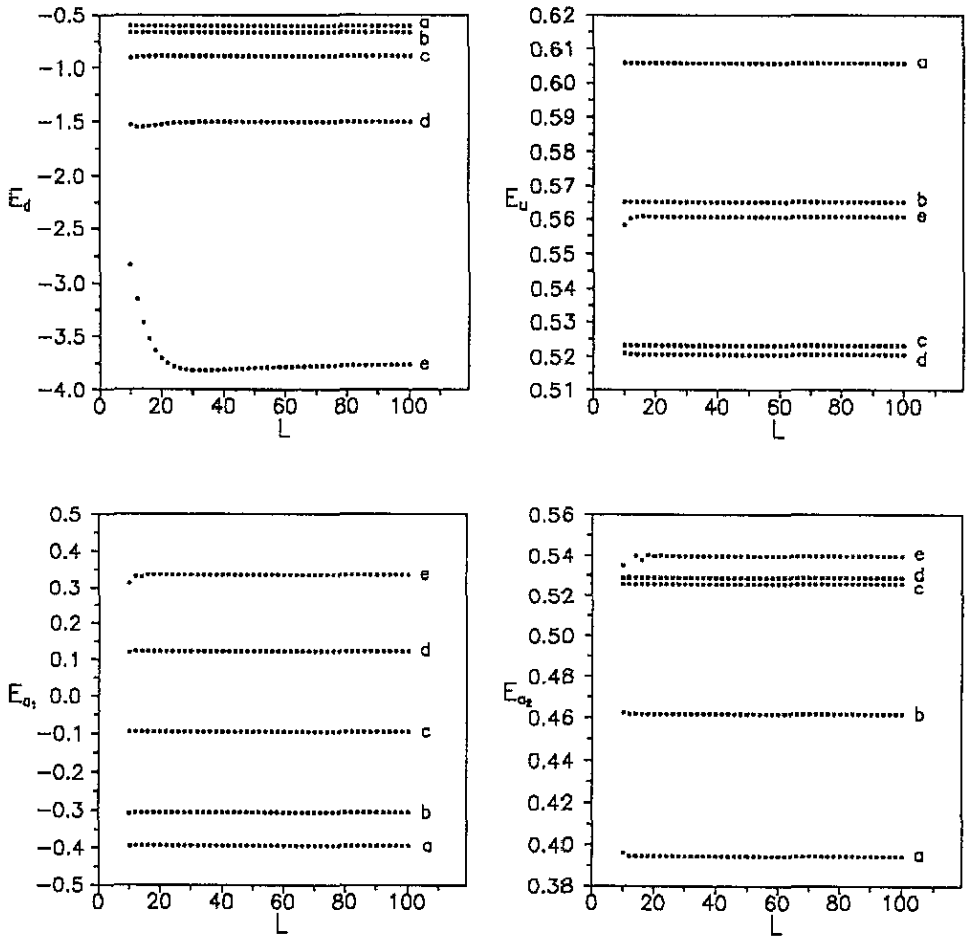

Figure 5. The L-dependence of the exact numerical bounds of the fully occupied (E_d), completely empty (E_u) lattice and the chessboard configuration (E_{a_1}, E_{a_2}) calculated for $U = 3$ and (*a*) $q = 0$, (*b*) $q = 0.1$, (*c*) $q = 0.3$, (*d*) $q = 0.5$ and (*e*) $q = 0.7$.

Figure 6 presents results obtained for a finite system of 240 sites. It is seen that all our observations made on small systems also hold for much larger systems, and even some features of the valence transitions are now more visible. For example, it is evident that for all values of q the valence transitions have their own internal structure. The most homogeneous configurations with $n_f = 1 - 1/i$ ($E < 0$) or $n_f = 1/i$ ($E > 0$), $i = 1, 2 \ldots L$ form the primary structure, depending on L only very weakly, while the remaining most homogeneous configurations form the secondary structure, which depends very strongly on L and U. However, with increasing U (for fixed q) the secondary structure is gradually suppressed and only the primary structure forms the transition. For sufficiently large U this structure is very simple and consists of a few relevant transitions, whose number can be further reduced by q. This means that in the pressure-induced case the spinless Falicov–Kimball model undergoes only a few (discrete) intermediate-valence transitions, namely the transitions from an integer-valence ground state into an inhomogeneous intermediate-

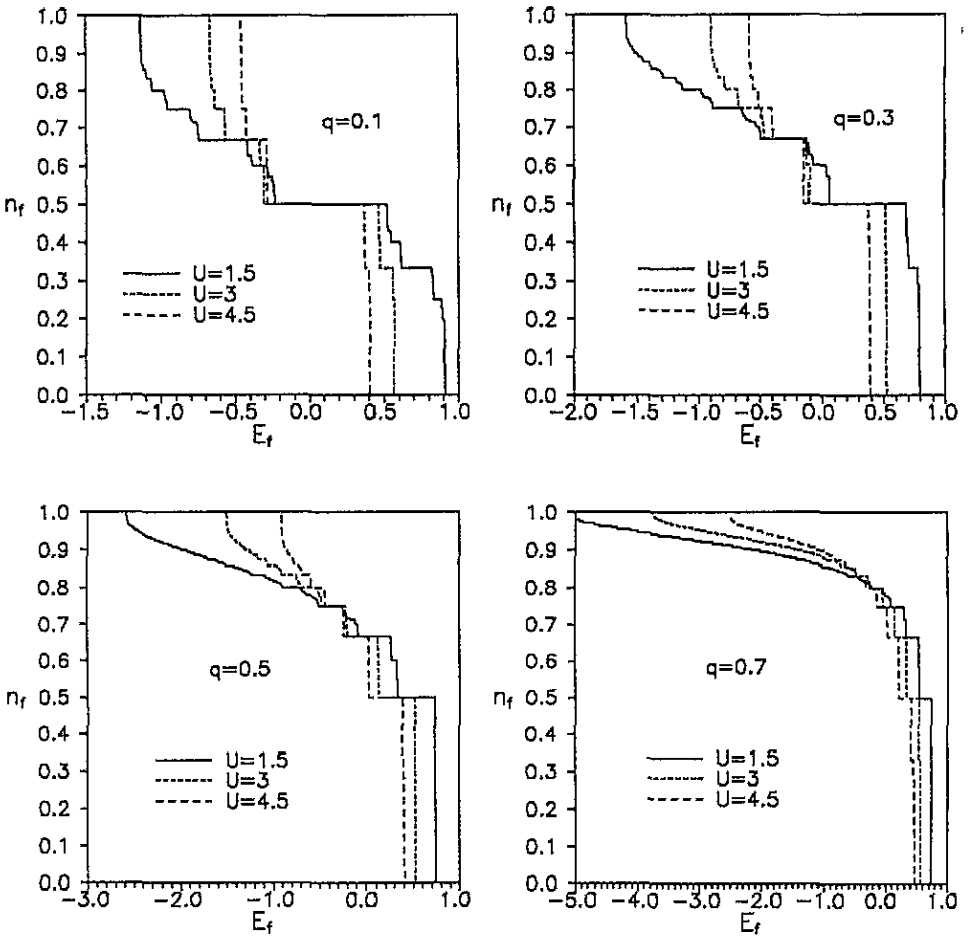

Figure 6. The dependence of the f-electron occupation density n_f (calculated for the most homogeneous configurations) on the f-level position E_f for $L = 240$, $U = 1.5, 3, 4.5$ and $q = 0.1$, 0.3, 0.5 and 0.7.

valence state† and the transitions from one inhomogeneous intermediate-valence state into another inhomogeneous intermediate-valence state. The effect of q is particularly strong for $n_f \leqslant 0.5$, where even for relatively small values of U the number of relevant transitions is reduced at sufficiently large q ($q \simeq 0.5$) to one: from $n_f = 1/2$ to 0 (see figures 3 and 4). Since the primary structure is almost independent of finite-size effects we suppose that this picture of the valence transitions in the framework of the Falicov–Kimball model could be very close to the real one.

It should be noted that our picture of valence transitions based on the exact numerical calculations differs strongly from the picture obtained so far using various approximations. Whereas our results predict that the spinless Falicov–Kimball model undergoes a few

† In the rare-earth community the concept of an 'inhomogeneous intermediate-valence state' is used to denote the static mixture of rare-earth ions with valence n or $n-1$ depending on the lattice site. This is in contrast to the dynamical mixture (homogeneous mixed valence) when each rare-earth site looks identical in a time average, while the local state is best described by n at one time and $n-1$ at another. To avoid a misunderstanding, these concepts should be carefully distinguished from the concept of the most homogeneous configuration.

(discrete) intermediate-valence transitions, approximate solutions lead to very controversial and unreliable results, showing one or even no discontinuous valence transitions. The only fully reliable result seems to be the exact result of Brandt and Schmidt [4], obtained using Tchebycheff–Markov inequalities, which in the region where the authors are able to give exact numerical bounds yields the same structure as our results for $q \to 0$. This indicates that for $q \to 0$ approximate methods are not particularly appropriate for a description of valence and metal–insulator transitions, since these are very sensitive to the approximation used. However some approximations, for example the coherent-potential approximation, can be successful in the opposite limit $q \to 1$ when, as has been shown using exact analytical calculations [28], the coherent-potential approximation becomes exact for sufficiently small values of U. Unfortunately, the limit $q = 1$ is not very realistic, since the entire kinetic energy of the system is now carried by one electron in the state $k = 0$, while the remaining electrons are immobile.

Finally, it should be mentioned that the picture presented of valence transitions is considerably simplified, and in more detailed analyses one must consider higher dimensions, larger lattices, electron–phonon interactions, orbital dynamics as well as the d–f hybridization. Work on this object is in progress, and preliminary results show that the fundamental features of transitions described above hold for higher dimensions and for larger lattices.

In summary, we have investigated the possibilities for intermediate-valence transitions in the one-dimensional spinless Falicov–Kimball model with a generalized type of hopping. We found that the valence transitions have a staircase structure almost independent of finite-size effects, which is maximally simplified with increasing U and q. Thus for sufficiently large U and q the Falicov–Kimball model undergoes, in the pressure-induced case, only a few discrete intermediate-valence transitions, namely the transitions from an integer-valence ground state into an inhomogeneous intermediate-valence state and the transitions from one inhomogeneous intermediate-valence state into another inhomogeneous intermediate-valence state.

References

[1] Falicov L M and Kimball J C 1969 *Phys. Rev. Lett.* **22** 997
[2] Kennedy T and Lieb E H 1986 *Physica* A **138** 320
[3] Hubbard J 1963 *Proc. R. Soc.* A **276** 238
[4] Brandt U and Schmidt R 1986 *Z. Phys.* B **63** 45; 1987 *Z. Phys.* B **67** 43
[5] Brandt U and Mielsch C 1989 *Z. Phys.* B **75** 365; 1990 *Z. Phys.* B **79** 295; 1991 *Z. Phys.* B **82** 37
Janiš V 1991 *Z Phys.* B **83** 227
van Dongen P G J and Vollhardt D 1991 *Phys. Rev. Lett.* **65** 1663
van Dongen P G J 1992 *Phys. Rev.* B **45** 2267
Freericks J K 1993 *Phys. Rev.* B **47** 9263
[6] Gruber Ch 1991 *Helv. Phys. Acta* B **64** 668
[7] Lyzwa R 1993 *Physica* A **192** 231
[8] Lemberger P 1992 *J. Phys. A: Math. Gen.* **25** 715
[9] Gruber Ch, Lebowitz J L and Macris N 1993 *Europhys. Lett.* **21** 389; 1993 *Phys. Rev.* B **48** 4312
[10] Goncalves da Silva C E T and Falicov L M 1972 *J. Phys. C: Solid State Phys.* **9** 906
[11] Rossler J and Ramirez R 1976 *J. Phys. C: Solid State Phys.* **9** 3747
[12] Schweitzer J W 1977 *Phys. Rev.* B **17** 758
[13] Plischke M 1972 *Phys. Rev. Lett.* **28** 361
[14] Ghosh D K 1976 *Solid State Commun.* **18** 1377
[15] Hewson A C and Reiseborough P S 1977 *Solid State Commun.* **22** 379
[16] Avignon M and Ghatak S K 1975 *Solid State Commun.* **16** 1243
[17] Goncalves da Silva C E T and Falicov L M 1975 *Solid State Commun.* **17** 1521

[18] Kanda K, Machida K and Matsubara T 1976 *Solid State Commun.* **19** 651
[19] Leder H J 1978 *Solid State Commun.* **27** 579
[20] Iglesias-Sicardi J R and Aveline I 1980 *Solid State Commun.* **36** 19
[21] Singh I, Abuja A K and Joshi S K 1980 *Solid State Commun.* **34** 65
[22] Baeck E and Czycholl G 1982 *Solid State Commun.* **43** 89
[23] Farkašovský P 1994 *Phys. Rev.* B at press
[24] Farkašovský P 1992 *Mod. Phys. Lett.* B **6** 793
[25] Farkašovský P and Batko I 1993 *J. Phys.: Condens. Matter* **5** 7131
[26] Freericks J K and Falicov L M 1990 *Phys. Rev.* B **41** 2163
[27] Horn R A and Johnson Ch R 1986 *Matrix Analysis* (Cambridge: Cambridge University Press)
[28] Farkašovský P 1993 *Czech. J. Phys.* **43** 159