IOPscience iopscience.iop.org

Home Search Collections Journals About Contact us My IOPscience

Insulator-metal transitions in the Falicov-Kimball model with a generalized type of hopping

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

1995 J. Phys.: Condens. Matter 7 9775

(http://iopscience.iop.org/0953-8984/7/50/012)

View the table of contents for this issue, or go to the journal homepage for more

Download details:
IP Address: 171.66.16.151
The article was downloaded on 12/05/2010 at 22:44

Please note that terms and conditions apply.

J. Phys.: Condens. Matter 7 (1995) 9775–9783. Printed in the UK

Insulator–metal transitions in the Falicov–Kimball model with a generalized type of hopping

Pavol Farkašovský

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

Received 2 May 1995, in final form 10 October 1995

Abstract. The possibilities for the insulator–metal transitions in the spinless Falicov–Kimball model with a generalized type of hopping are studied using small-cluster exact diagonalization calculations. It is shown that for small values of the interaction strength U the energy gap Δ vanishes discontinuously at some critical value of the f-electron occupation number and thus in the pressure-induced case the model can describe the insulator–metal transition observed in some rare-earth compounds.

In our preceding paper [1] we studied valence transitions in the spinless Falicov–Kimball model with a generalized type of hopping. We found that even for relatively small values of the interaction strength U the basic structure of the valence transition can be described very precisely taking into account only the most homogeneous configurations. For this set of configurations the model undergoes only a few discrete intermediate-valence transitions and thus in the pressure-induced case when the f-level position is pushed upward it could describe the discontinuous intermediate-valence transitions observed in some rare-earth compounds [2]. Unfortunately due to the replacement of the real ground-state configurations by the most homogeneous configurations we were not able to decide whether the discontinuous intermediate-valence transitions obtained are insulator–metal transitions or only insulator–insulator transitions. To resolve this important problem satisfactorily we have in the present paper extended our early small-cluster exact diagonalization calculations with a more exhaustive numerical study of the model. We have found that the Falicov–Kimball model can be used to describe both of the above-mentioned types of transition and thus it seems to be a convenient model for a description of the valence and insulator–metal transitions in some rare-earth and transition-metal compounds [2].

The model to be discussed in this paper is identical to the one used in the previous paper [1] :

$$H = \sum_{ij} t_{ij}(q) d_i^+ d_j + U \sum_i w_i d_i^+ d_i + E_f \sum_i w_i \tag{1}$$

where d_i^+ (d_i) are the creation (annihilation) operators of the itinerant spinless electrons in the d-band Wannier state at site i and w_i is the occupation number of the localized f electrons taking the value 1 or 0 according to whether the site i is occupied or unoccupied by an f electron.

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 the nearest neighbours and zero otherwise; however, to study effects of the band

0953-8984/95/509775+09$19.50 © 1995 IOP Publishing Ltd

on the valence and insulator–metal transitions we adopt the following general form of the matrix elements:

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

which represents a much more realistic type of hopping.

The second term is the on-site Coulomb interaction between the d-band electrons with density

$$n_d = (1/L)\sum_i d_i^+ d_i$$

and the localized f electrons with density

$$n_f = (1/L)\sum_i w_i$$

where L is the number of lattice sites. The third term stands for the localized f electrons whose sharp energy level is E_f.

For a given f-electron configuration $w = \{w_1, w_2, \ldots, w_L\}$ defined on the one-dimensional lattice with periodic boundary conditions, the Hamiltonian (1) is the second-quantized version of the single-particle Hamiltonian $h(w) = T + UW$, whose matrix elements are $h_{ij} = t_{ij} + Uw_i\delta_{ij}$, and thus the investigation of the model (1) 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 proceed directly in the following steps (next we consider just the case where $N_f + N_d = L$, which is of special interest for the mixed-valence phenomena): (1) having U, E_f, q and $w = \{w_1, w_2, \ldots, w_L\}$ fixed, find all the eigenvalues λ_k of $h(w) = T + UW$; (2) 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; (3) find w^0 for which $E(w, U, E_f)$ has a minimum. Now 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 or E_f respectively. It should be noted that this problem, and particularly the question of whether the Falicov–Kimball model can or cannot 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 [3] that the external pressure shifts the energy level E_f, then the valence transitions observed in some rare-earth compounds (SmB_6, SmS, TmTe, etc) could be understandable purely electronically, if $n_f(E_f)$ really has discontinuities.

To show qualitatively the possibilities for the insulator–metal transitions in the spinless Falicov–Kimball model with a generalized type of hopping let us first examine the ground-state phase diagram of the model on a finite one-dimensional lattice of 20 sites. The exact numerical results obtained for a complete set of 2^{20} f-electron configurations are shown in figure 1 and figure 2 for two different values of q and $E_f = 0$. It should be noted that we can restrict our investigation of the possibilities for the insulator–metal transitions to the case where $U < U_0 = 4/(1-q^2)$ since, by a theorem of Gersgorin [4], there is always a finite gap in the spectrum of $h(w)$ for $U > U_0$ and $N_d + N_f = L$.

Figure 1 presents the ground-state phase diagram for $q = 0.1$. Our exact numerical results indicate that the phase diagram of the Falicov–Kimball model with a generalized

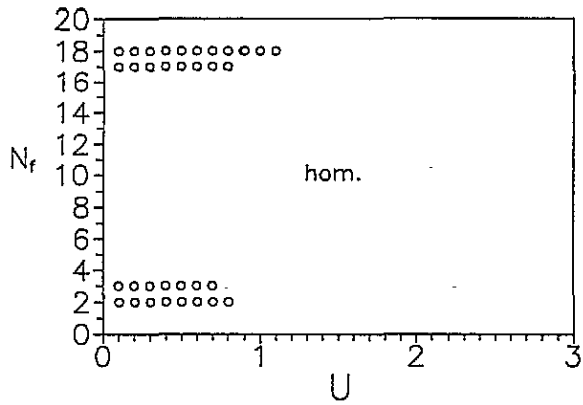

Figure 1. The ground-state phase diagram of the spinless Falicov–Kimball model with a generalized type of hopping for $q = 0.1$ and $L = 20$. In the region denoted hom. the ground states are the most homogeneous configurations, while in the regions denoted with ∘ the ground states are mixtures of the empty ($n_f \to 0$) or the fully occupied ($n_f \to 1$) configuration and some configuration w.

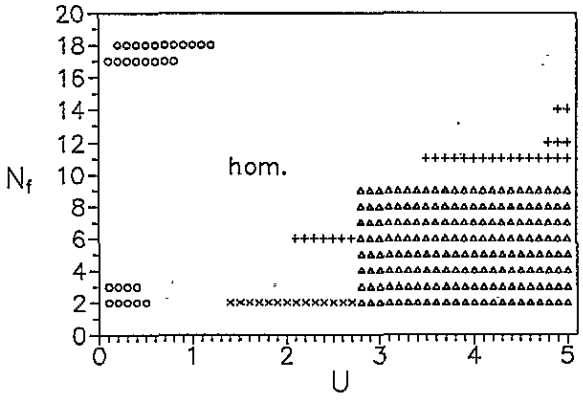

Figure 2. The ground-state phase diagram for $q = 0.3$ and $L = 20$. The phase Δ corresponds to mixtures of the alternating configurations $w_a(N_f)$ with the empty configuration, while in the phase $\times$ ($N_f = 2$) the ground-state configuration varies gradually from the most homogeneous to $\{101000\ldots0\}$. In the configurations denoted as + the f electrons are distributed similarly to in the most homogeneous configurations, i.e., the distances between two consecutive f electrons are either d or $d + 1$; however, the most homogeneous distribution of distances d and $d + 1$ is broken here.

type of hopping is separated into several distinct regions. In the first region the most homogeneous configurations are the ground states. In the second region ($U < 1, n_f \to 0$) the ground states are configurations each consisting of at least $L/2$ consecutive unoccupied sites (they can be considered as mixtures of the empty configuration and some configuration w), and in the third region ($U < 1, n_f \to 1$) configurations consisting of at least $L/2$ consecutive occupied sites minimize the ground-state energy. For example, for $N_f = 2$ the ground state is the configuration $1_2 0_{18}$ consisting of 2 occupied sites followed by 18 unoccupied sites, and for $N_f = 3$ the ground state is the configuration $1_2 0_4 1_1 0_{13}$ (the subscript denotes the number of consecutive sites occupied (unoccupied) by f electrons). These results indicate that, for $U < 1$ and sufficiently small (large) f-electron densities, the

ground-state configurations could be mixtures of two configurations, one of which is the empty (fully occupied) configuration. Figure 3 shows that the ground states corresponding to the most homogeneous configurations are insulating since for all these configurations the energy gap Δ at the Fermi level E_F [5] has a finite width. Thus the only possible candidates for the insulator–metal transitions are the small regions near $n_f = 0$ and $n_f = 1$, where the ground states are mixtures of the empty (fully occupied) configuration and some configuration w. If this separation persists on much larger lattices, we can indeed expect metallic behaviour in these regions since the Fermi level of such mixtures is located in the band of the empty configuration, and therefore an extra electron can be added at no energy cost. Our numerical results presented in the following fully accord with this physical expectation. Before discussing these results let us show how this picture changes with increasing q.

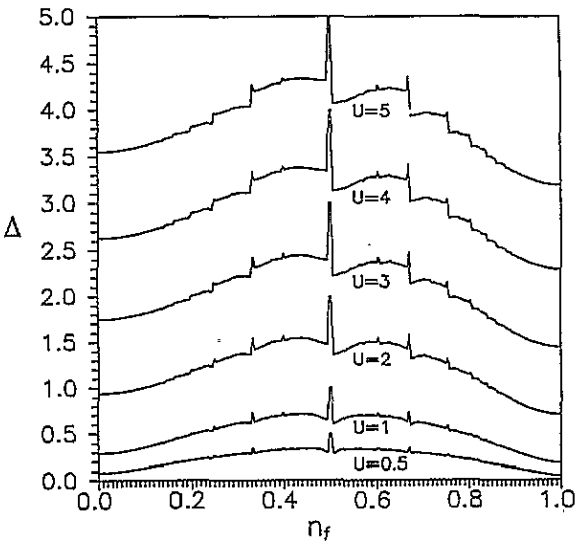

Figure 3. The n_f-dependence of the energy gap Δ calculated for the most homogeneous configurations at six different values of U and for $q = 0.1$, $L = 240$.

Figure 2 presents the situation for $q = 0.3$. We can see that the largest region of stability still corresponds to the most homogeneous configurations; however, in addition to this region and two small regions near $n_f = 0$ and $n_f = 1$ there appears now a new large region ($U \geqslant U_c = 2.783, n_f \leqslant 0.5$) where the configurations of the type $\{1010\ldots1000\ldots0\}$ (they can be considered as mixtures of the empty configuration and the alternating configuration $w_a(N_f) = \{1010\ldots\}$, with $N_f = 1, 2, \ldots, L/2$) are the ground states. Thus a further candidate for the insulator–metal transition is the region $U \geqslant U_c, n_f \leqslant 0.5$ and particularly its boundaries. However, illustrating the U-dependence of the energy gap calculated for different f-electron concentrations n_f and $L = 24$ (see figure 4, left panel), the energy gaps for all of the n_f have finite values below as well as above U_c and thus there is probably no insulator–metal transition at U_c. To verify this guess we have considered a much larger lattice of 240 sites. For $U = U_c$ we have calculated the energy gaps of all mixtures (alternating configuration + empty configuration) which are the ground states above U_c and all homogeneous configurations which are the ground states below U_c [6]. It is seen from figure 5 that going with n_f from 0 to 1 there is no insulator–metal transition at $n_f = 0.5$; nor is there an insulator–metal transition at U_c for any n_f. Although in both cases there

exist finite kinks, the energy gap is always nonzero and thus the insulator–metal transition is absent at $U = U_c$ and $n_f = 0.5$. Thus only the small regions near $n_f = 0$ and $n_f = 1$ remain candidates for the insulator–metal transition. Indeed, already results on the small lattices (see figure 4, right-hand panel) indicate that this conjecture would hold true. Therefore, we now turn our attention fully to these regions.

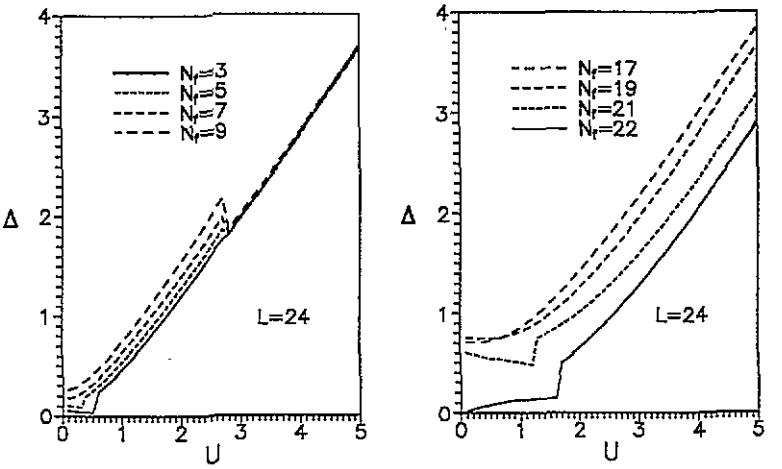

Figure 4. The U-dependence of the energy gap for $q = 0.3$ and $L = 24$.

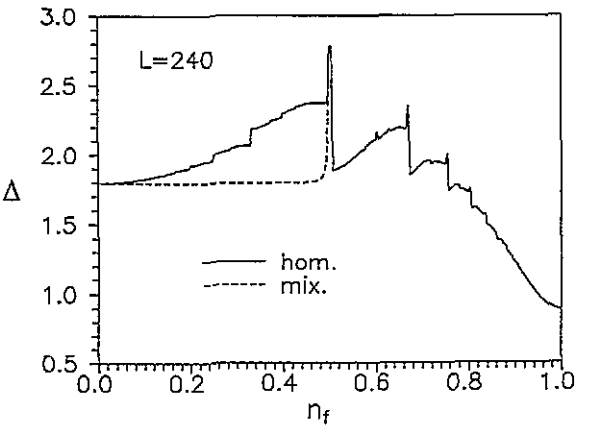

Figure 5. The n_f-dependence of the energy gap calculated for the most homogeneous configurations (solid line) and the mixtures of the alternating configurations $w_a(N_f)$ with the empty configuration (dashed line). $L = 240$, $U = 2.783$, $q = 0.3$.

The exact numerical results obtained for $U = 0.6$ and a complete set of configurations on small finite lattices are summarized in tables 1 and 2. We have found that independently of L there exist critical values of the f-electron occupation number N_{c_1} and N_{c_2} such that for $N_{c_1} \leqslant N_f \leqslant N_{c_2}$ the ground states are the most homogeneous configurations, while for $N_f \leqslant N_{c_1}$ ($N_{c_2} < N_f \leqslant L$) the ground states are mixtures of the empty (fully occupied) configuration and some configuration w (see tables 1 and 2). It is seen that the values of N_{c_1} and N_{c_2} decrease with increasing q and the region of possible insulator–metal transitions is reduced consequently. For $q > 0.6$ this region practically disappears. The long-range

Table 1. The critical values of the f-electron occupation number N_{c_1} and the ground-state configurations (g.s.c.) below N_{c_1} calculated for $U = 0.6$ and different values of L. Here the subscript denotes the number of consecutive sites occupied (unoccupied) by f electrons in a g.s.c.

L	N_c	$q = 0.1$	N_c	$q = 0.2$
16	2	$1_2 0_{14}$		
18	3	$1_2 0_{16}$, $1_2 0_4 1_1 0_{11}$	2	$1_2 0_{16}$
20	3	$1_2 0_{18}$, $1_2 0_4 1_1 0_{13}$	2	$1_2 0_{18}$
22	3	$1_2 0_{20}$, $1_2 0_4 1_1 0_{15}$	3	$1_2 0_{20}$, $1_2 0_4 1_1 0_{15}$
24	3	$1_2 0_{22}$, $1_2 0_5 1_1 0_{16}$	3	$1_2 0_{22}$, $1_2 0_4 1_1 0_{17}$
26	4	$1_2 0_{24}$, $1_2 0_5 1_1 0_{18}$ $1_2 0_3 1_2 0_{19}$	3	$1_2 0_{24}$, $1_2 0_5 1_1 0_{18}$
28	4	$1_2 0_{26}$, $1_2 0_5 1_1 0_{20}$ $1_2 0_3 1_2 0_{21}$	4	$1_2 0_{26}$, $1_2 0_5 1_1 0_{20}$ $1_1 0_4 1_2 0_4 1_1 0_{16}$
30	5	$1_2 0_{28}$, $1_2 0_6 1_1 0_{21}$ $1_2 0_3 1_2 0_{23}$, $1_2 0_3 1_2 0_4 1_1 0_{18}$	4	$1_2 0_{28}$, $1_2 0_5 1_1 0_{22}$ $1_2 0_3 1_2 0_{23}$
32	5	$1_2 0_{30}$, $1_2 0_6 1_1 0_{23}$ $1_2 0_4 1_2 0_{24}$, $1_2 0_3 1_2 0_4 1_1 0_{20}$	4	$1_2 0_{30}$, $1_2 0_5 1_1 0_{24}$ $1_2 0_3 1_2 0_{25}$
34	5	$1_2 0_{32}$, $1_2 0_6 1_1 0_{25}$ $1_2 0_4 1_2 0_{26}$, $1_2 0_3 1_2 0_4 1_1 0_{22}$	5	$1_2 0_{32}$, $1_2 0_5 1_1 0_{26}$ $1_2 0_3 1_2 0_{27}$, $1_1 0_4 1_2 0_4 1_1 0_4 1_1 0_{17}$
36	5	$1_2 0_{34}$, $1_2 0_7 1_1 0_{26}$ $1_2 0_4 1_2 0_{28}$, $1_2 0_3 1_2 0_4 1_1 0_{24}$	5	$1_2 0_{34}$, $1_2 0_6 1_1 0_{27}$ $1_2 0_3 1_2 0_{29}$, $1_2 0_3 1_2 0_4 1_1 0_{24}$
48	8	$1_2 0_{46}$, $1_1 0_8 1_2 0_{37}$ $1_2 0_5 1_2 0_{39}$, $1_2 0_4 1_2 0_6 1_1 0_{33}$ $1_2 0_4 1_2 0_4 1_2 0_{34}$, $1_2 0_3 1_2 0_3 1_2 0_4 1_1 0_{31}$ $1_2 0_3 1_2 0_3 1_2 0_4 1_1 0_4 1_1 0_{26}$	7	$1_2 0_{46}$, $1_1 0_6 1_2 0_{39}$ $1_2 0_4 1_2 0_{40}$, $1_2 0_4 1_2 0_5 1_1 0_{34}$ $1_2 0_3 1_2 0_3 1_2 0_{36}$, $1_2 0_3 1_2 0_3 1_1 0_5 1_1 0_5 1_1 0_{24}$

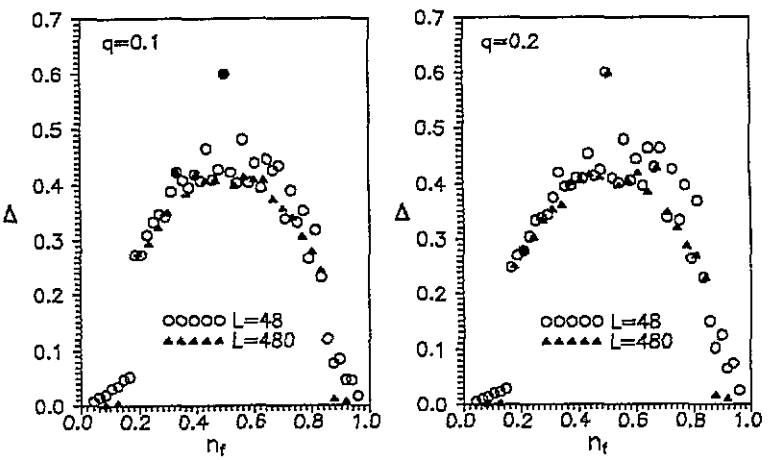

Figure 6. The n_f-dependence of the energy gap calculated for $q = 0.1$ and $q = 0.2$. Circles correspond to $L = 48$ and triangles to $L = 480$.

hopping stabilizes the insulating state. Note that our exact analytical calculations [7] performed in the limit $q \to 1$ fully confirm this result.

The n_f-dependence of the energy gap calculated for the largest finite lattice ($L = 48$) which we have been able to solve for numerically is plotted in figure 6. Although the results are still affected by an error due to the finite-size effects they apparently show that below N_{c_1} (above N_{c_2}) the gap is suppressed and vanishes probably discontinuously. To

Table 2. The critical values of the f-electron occupation number N_{c_2} and the ground-state configurations above N_{c_2} calculated for $U = 0.6$ and different values of L. For $L = 48$ the results have been computed only for $q = 0.1$ and $q = 0.2$.

L	N_c	$q = 0.1$	N_c	$q = 0.2$	N_c	$q = 0.3$
16	14	$0_2 1_{14}$				
18	15	$0_2 1_{16}$	15	$0_2 1_{16}$	16	$0_2 1_{16}$
		$0_2 1_4 0_1 1_{11}$		$0_2 1_4 0_1 1_{11}$		
20	17	$0_2 1_{18}$	17	$0_2 1_{18}$	17	$0_2 1_{18}$
		$0_2 1_5 0_1 1_{12}$		$0_2 1_5 0_1 1_{12}$		$0_2 1_5 0_1 1_{12}$
22	19	$0_2 1_{20}$	19	$0_2 1_{20}$	19	$0_2 1_{20}$
		$0_2 1_5 0_1 1_{14}$		$0_2 1_5 0_1 1_{14}$		$0_2 1_5 0_1 1_{14}$
24	21	$0_2 1_{22}$	21	$0_2 1_{22}$	21	$0_2 1_{22}$
		$0_2 1_6 0_1 1_{15}$		$0_2 1_6 0_1 1_{15}$		$0_2 1_6 0_1 1_{15}$
26	22	$0_2 1_{24}$	23	$0_2 1_{24}$	23	$0_2 1_{24}$
		$0_2 1_6 0_1 1_{17}$		$0_3 1_{23}$		$0_3 1_{23}$
		$0_2 1_4 0_2 1_{18}$				
28	23	$0_2 1_{26}$	24	$0_2 1_{26}$	25	$0_2 1_{26}$
		$0_3 1_{25}$		$0_3 1_{25}$		$0_3 1_{25}$
		$0_2 1_4 0_2 1_{20}$		$0_2 1_4 0_2 1_{20}$		
		$0_1 1_4 0_2 1_3 0_2 1_{16}$				
30	25	$0_2 1_{28}$	25	$0_2 1_{28}$	26	$0_2 1_{28}$
		$0_3 1_{27}$		$0_3 1_{27}$		$0_3 1_{27}$
		$0_2 1_4 0_2 1_{22}$		$0_2 1_5 0_2 1_{21}$		$0_2 1_5 0_2 1_{21}$
		$0_2 1_3 0_2 1_4 0_1 1_{18}$		$0_2 1_4 0_2 1_4 0_1 1_{17}$		
32	27	$0_2 1_{30}$	27	$0_2 1_{30}$	27	$0_2 1_{30}$
		$0_3 1_{29}$		$0_3 1_{29}$		$0_3 1_{29}$
		$0_2 1_5 0_2 1_{23}$		$0_2 1_5 0_2 1_{23}$		$0_2 1_5 0_2 1_{23}$
		$0_2 1_4 0_2 1_4 0_1 1_{19}$		$0_2 1_4 0_2 1_4 0_1 1_{19}$		$0_2 1_4 0_2 1_5 0_1 1_{18}$
34	29	$0_2 1_{32}$	29	$0_2 1_{32}$	29	$0_2 1_{32}$
		$0_3 1_{31}$		$0_3 1_{31}$		$0_3 1_{31}$
		$0_2 1_5 0_2 1_{25}$		$0_2 1_5 0_2 1_{25}$		$0_2 1_6 0_2 1_{24}$
		$0_2 1_4 0_2 1_5 0_1 1_{20}$		$0_2 1_4 0_2 1_5 0_1 1_{20}$		$0_2 1_4 0_2 1_5 0_1 1_{20}$
36	30	$0_2 1_{34}$	31	$0_2 1_{34}$	31	$0_2 1_{34}$
		$0_3 1_{33}$		$0_3 1_{33}$		$0_3 1_{33}$
		$0_2 1_5 0_2 1_{27}$		$0_2 1_6 0_2 1_{26}$		$0_2 1_6 0_2 1_{26}$
		$0_2 1_4 0_2 1_5 0_1 1_{22}$		$0_2 1_4 0_2 1_5 0_1 1_{22}$		$0_2 1_5 0_2 1_5 0_1 1_{21}$
		$0_1 1_4 0_2 1_3 0_2 1_4 0_1 1_{19}$				
48	41	$0_2 1_{46}$	41	$0_2 1_{46}$		
		$0_3 1_{45}$		$0_3 1_{45}$		
		$0_2 1_7 0_2 1_{37}$		$0_2 1_8 0_2 1_{36}$		
		$0_1 1_7 0_2 1_6 0_2 1_{30}$		$0_2 1_5 0_3 1_{38}$		
		$0_2 1_5 0_2 1_5 0_2 1_{32}$		$0_2 1_5 0_2 1_5 0_2 1_{32}$		
		$0_2 1_4 0_2 1_4 0_2 1_5 0_1 1_{28}$		$0_2 1_4 0_2 1_4 0_2 1_5 0_1 1_{28}$		

confirm this conjecture and to exclude the finite-size effects we have computed the energy gaps of selected configurations on a much larger lattice of 480 sites. For our numerical results obtained on small lattices we have chosen the following set of configurations: (i) for $N_{c_1} \leqslant N_f \leqslant N_{c_2}$ the most homogeneous configurations; (ii) below $N_f < N_{c_1}$ (above $N_f > N_{c_2}$) the mixtures of the empty (fully occupied) configuration with $[1_2 0_5]$, $[1_2 0_4]$ ($[0_2 1_7]$, $[0_2 1_5]$) configurations [8] for $q = 0.1$ and $[1_2 0_4]$, $[1_2 0_3]$ ($[0_2 1_8]$, $[0_2 1_5]$) configurations for $q = 0.2$, which are the ground states on larger lattices for $n_f = \frac{1}{12}, \frac{1}{8}$ ($n_f = 1 - \frac{1}{12}, 1 - \frac{1}{8}$) (see tables 1 and 2). The energy gaps calculated for these configurations correlate very well with the exact numerical results obtained for $L = 48$ and thus we expect

that the real picture of the insulator–metal transition would be very close to this one. For $N_{c_1} < N_f < N_{c_2}$ the gap has a finite width, while below N_{c_1} (above N_{c_2}) the gap vanishes–the insulator–metal transition takes place at N_{c_1} (N_{c_2}).

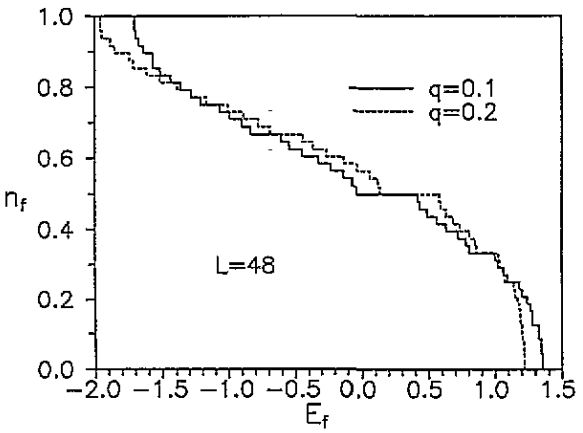

Figure 7. The dependence of the f-electron occupation density n_f on the f-level position E_f for $L = 48$, $q = 0.1$ (solid line) and $q = 0.2$ (dashed line).

As we have discussed in our previous paper [1] (see also figure 7) the change of n_f can be induced by the shift of the f-level position E_f. However, this shift, on the other hand, can be driven by external pressure p, so we have the discontinuous insulator–metal transition in the spinless Falicov–Kimball model at $E_f = E_c$ ($p = p_c$). Such behaviour of the energy gap with the external pressure was really observed recently by Colley *et al* [9] for SmB_6. Performing a more exhaustive resistivity study also supplemented by Hall effect measurements, they found that the energy gap does not vanish continuously as the previous resistivity studies indicated [10] but vanishes discontinuously at ~50 kbar. Thus, taking into account our present as well as previous results [1, 11] we can conclude that the Falicov–Kimball model is indeed a convenient model for description of the valence and insulator–metal transitions in rare-earth compounds, since it apparently supports both discontinuous intermediate–valence transitions as a function of E_f [1], and discontinuous metal–insulator transitions as a function of n_f. Since, in practice n_f is a function of E_f, the comprehensive picture of valence and metal–insulator transitions in the framework of the Falicov–Kimball model with a generalized type of hopping is as follows. In the strong-coupling limit the model undergoes a few discontinuous intermediate-valence transitions [1]. These 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 (at least for small values of q) [1, 11]. In the weak-coupling limit the basic structure of the transition is again formed by the most homogeneous configurations with the smallest periods; however, the transitions between two such configurations (unlike in the case of large U) are now gradual (see figure 7). In addition, for sufficiently small U and $n_f \to 0$ or 1 the energy gap vanishes discontinuously at $n_f = n_{c_1}$ and $n_f = n_{c_2}$ ($E_f = E_{c_1}, E_{c_2}$) and thus discontinuous insulator–metal transitions take place at these points. The values of n_{c_1} and n_{c_2} decrease with increasing q and the accessible regions of insulator–metal transitions are consequently reduced. For sufficiently large values of q ($q > 0.6$) these regions practically disappear.

Acknowledgments

This work was partially supported by the Slovak Grant Agency for Science and the Commission of the European Communities Contract No ERB CHRX CT93.0115 (subcontract ERB CIPD CT94.0030).

References

[1] Farkašovský P 1995 *J. Phys.: Condens. Matter* **7** 3001
[2] Khomskii D L 1982 *Quantum Theory of Solids* ed I M Lifshitz (Moscow: Mir)
[3] Goncalves da Silva C E T and Falicov L M 1975 *Solid State Commun.* **17** 1521
[4] Horn R A and Johnson C R 1986 *Matrix Analysis* (Cambridge: Cambridge University Press)
[5] Since we consider the case where $N_f + N_d = L$, the Fermi level E_F and the energy gap Δ of some configuration w are given by $E_F = \lambda_{L-N_f}$ and $\Delta = \lambda_{L-N_f+1} - \lambda_{L-N_f}$, respectively.
[6] Considering the most homogeneous configurations instead of mixtures which are the ground states below U_c for some N_f does not change the picture presented, since the energy gaps corresponding to these configurations lie between the energy gaps of the most homogeneous configurations and the alternating configurations $w_\alpha(N_f)$.
[7] Farkašovský P 1992 *Mod. Phys. Lett.* B **6** 1245
[8] $[1_p 0_m]$ denotes the unit cell of the configuration.
[9] Colley J C, Aronson M C, Fisk Z and Canfield P C 1995 *Phys. Rev. Lett.* **74** 1629
[10] Moshchalkov V V, Berman I V, Brandt M B, Pashkevich S M, Bogdanov E V, Konovalova E S and Semenov M V 1985 *J. Magn. Magn. Mater.* **47–48** 289
[11] Farkašovský P 1995 *Phys. Rev.* B **51** 1507