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Ground states of the spinless Falicov–Kimball model in the strong-coupling limit

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Abstract. We have studied energetic and structural ground-state properties of the one-dimensional Falicov–Kimball model in the strong-coupling limit. Using standard perturbation theory we recover some results already obtained (the phase segregation at large interactions) and we present some new results concerning the ground state, e.g., the analytic expression for the boundary, below which the segregated configuration cannot be the ground state, and the phase diagram of the model calculated for special periodic (aperiodic) configurations of ions and for the case when the ion concentration goes to zero.

1. Introduction

The study of electron correlation effects induced by strong, short-ranged interactions in Fermi systems is surely at the centre of interest of contemporary solid-state physics. The motivation is clearly due to discoveries of new materials such as the heavy-fermion compounds or the high-temperature superconductors, to mention only two. Meanwhile it is generally accepted that most of the quite unusual properties of these materials such as itinerant magnetism, metal–insulator transitions, metallic crystallization, superconductivity etc, are caused by the strongly correlated electrons. Systems of this kind are usually described by fermionic lattice models, i.e., models with itinerant quantum-mechanical degrees of freedom. The simplest model of this type is the Falicov–Kimball model introduced more than two decades ago [1].

The one-band spinless version of the Falicov–Kimball model is defined by the following Hamiltonian:

$$H = \sum_{i,j} t_{i,j} c_i^+ c_j + U \sum_i w_i c_i^+ c_i \tag{1}$$

where c_i^+ (c_i) are fermionic creation (annihilation) operators for the spinless electron at site i and w_i is the occupation number of the ions, taking the value 1 or 0 at each site according to whether the site i is occupied or unoccupied, respectively, by an ion.

The kinetic energy (the first term of (1)) is due to quantum-mechanical hopping of electrons between sites i and j, and these intersite hopping transitions are described by the general matrix element $t_{i,j}$. For the conventional Falicov–Kimball model it is usually assumed that $t_{i,j} = -t$ if i and j are nearest neighbours and $t_{i,j} = 0$ otherwise. The second term represents an on-site interaction between electrons and ions that can be repulsive

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($U > 0$) or attractive ($U < 0$). In this model both the total electron number N_e and the total ion number N_i defined by

$$N_e = \sum_i c_i^+ c_i \qquad N_i = \sum_i w_i \tag{2}$$

are conserved quantities.

The Falicov–Kimball model was originally introduced [1] to study mixed-valence states in rare-earth compounds. There moving particles play the role of band s electrons and ions the role of f electrons. It can be also discussed as an approximation to the full Hubbard model [2], in which only up-spin electrons are allowed to hop and down-spin electrons are infinitely massive. Moreover, it was considered by Kennedy and Lieb [3] as a model for crystallization. In spite of its simplicity, so far only a few exact results concerning a ground state of the Hamiltonian (1) have been obtained.

(1) Brandt and Schmidt [4] using a method based on Tchebycheff–Markoff inequalities found sharp upper and lower bounds for the ground-state energy in two dimensions.

(2) Using the same method Gruber *et al* [5] calculated the phase diagram of the model. They determined domains in the plane of chemical potentials of electrons and ions, where the following ion configurations may be ground states: the checkerboard configuration; the completely empty configuration and the fully occupied configuration.

(3) Kennedy and Lieb [3] proved that the ground state has long-range order for all dimensions d.

(4) Recently, Brandt and Mielsch [6] obtained an exact solution in $d = \infty$.

(5) Freericks and Falicov [7] studied the model in one dimension (at present the exact solution of the model for $d = 1$ dimension does not exist). They presented the coherent and incoherent phase diagrams calculated numerically for the segregated phase and all periodic phases with periods less than nine and $N_i = \frac{1}{2}L, \frac{1}{3}L$, where L is the number of lattice sites. On the basis of these results they formulated a conjecture, the so-called segregation principle, which states the following: in the limit $|U/t| \to \infty$ the segregated phase, which is an incoherent mixture of the empty and full lattices with weights $(L - N_i)$ and N_i, is the ground state for all values of the electron concentration n_e except the specific values $n_e = 1 - n_i$ for $U/t \to \infty$ and $n_e = n_i$ for $U/t \to \infty$ ($n_e = N_e/L$, $n_i = N_i/L$).

(6) Brandt [8] was the first to analytically prove, that the segregation principle is true. He calculated the higher (lower) bound U^+ (U^-), above (below) which the segregated phase is (is not) the ground state of the one-dimensional Falicov–Kimball model. His results show that even for reasonably large deviations from the singular point $n_e/(1 - n_i) = 1$ the values U^+ (this quantity is given more precisely) and U^- are extremely large.

In the following sections we use the standard perturbation theory [9] to analyse the structure of the ground-state phase diagram of the one-dimensional Falicov–Kimball model in the strong-coupling limit. In section 3 we recover some results already obtained by Freericks and Falicov [7] and Brandt [8] (e.g. the phase segregation at large U) and in section 4 we present some new results concerning the ground state of the model (the analytical expression for the boundary $U_c \equiv U^-$, below which the segregated configuration cannot be the ground state, the phase diagram of the model for some special periodic (aperiodic) configurations of ions, the phase diagram for $n_i \to 0$, etc).

2. General properties of the model

For later reference let us first recall some general properties of the Falicov–Kimball model. The Hamiltonian (1) can be rewritten in the more convenient form

$$H(w) = \sum_{ij} h_{ij}(w) c_i^+ c_j \tag{3}$$

where

$$h_{ij}(w) = t_{ij} + U w_i \delta_{ij}. \tag{4}$$

Thus for a given ion configuration $w = \{w_1, w_2, \ldots, w_L\}$ defined on the one-dimensional lattice of L sites with periodic boundary conditions, the Hamiltonian (3) is the second quantized version of the single-particle Hamiltonian

$$\mathbf{h}(w) = \mathbf{T} + U\mathbf{W} = \begin{pmatrix} Uw_1 & -t & 0 & \ldots & 0 & -t \\ -t & Uw_2 & -t & \ldots & 0 & 0 \\ 0 & -t & Uw_3 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & Uw_{L-1} & -t \\ -t & 0 & 0 & \ldots & -t & Uw_L \end{pmatrix} \tag{5}$$

so that the investigation of the model (1) is reduced to the investigation of the spectrum of $\mathbf{h}$, for different configurations of the ions.

In spite of its form the model considered is not one of independent particles, as it might be thought at first sight because w_i is allowed to vary and in the ground state with fixed values N_e and N_i, w_i must be chosen to minimize the ground-state energy

$$E_G(U, N_e, N_i) = \min\left(E(U, N_e, w) \Big| \sum_i w_i = N_i \right) \tag{6}$$

where $E(U, N_e, w)$ is the ground state energy for given N_e and w. (Here and for the remainder of the paper we use the energy scale in which all energies are measured in units of t.) Two well known particle–hole symmetries specific to the form of the Falicov–Kimball model, the ion-occupied–empty-site symmetry and an electron–hole symmetry, yield for $E(U, N_e, w)$ the following identities:

$$E(U, N_e, w^*) = E(-U, N_e, w) + UN_e \tag{7}$$

and

$$E(U, N_e, w) = E(-U, L - N_e, w) + UN_i. \tag{8}$$

The first relates ground states for the configuration $w = \{w_1, w_2, \ldots, w_L\}$ and for its conjugate configuration $w^* = \{1-w_1, 1-w_2, \ldots, 1-w_L\}$, and the second relates the ground states for N_e electrons and N_e holes. Using these symmetries we can restrict ourselves only to the case $U > 0$ and $N_e \leqslant N_i$, since the remaining cases may be deduced from a combination of (7) and (8).

3. Perturbative analysis; infinite U

To show some characteristic features and to define the basic concepts of the perturbation procedure of the one-dimensional Falicov–Kimball model in the strong-coupling limit let us start with the simplest case when $|U| \to \infty$. Let the interaction energy of the Hamiltonian (1) be the unperturbed Hamiltonian and let the kinetic energy be the perturbation. Because the matrix $\mathbf{W}$ is idempotent, the matrix $U\mathbf{W}$ has only two eigenvalues $E_1 = 0$ and $E_2 = U$. They are $(L - N_i)$-fold and N_i-fold degenerate and these degeneracies in consequence of a perturbation will have been completely or partly removed. The corresponding first-order corrections may be obtained using the standard perturbation theory of the degenerate levels [9]. The straightforward procedure for $E_1 = 0$ and $E_2 = U$ leads to the following secular equations:

$$E^{-N_i} \det[\mathbf{A}(w^*) - E\mathbf{I}] = 0 \tag{9}$$

$$E^{N_i - L} \det[\mathbf{A}(w) - E\mathbf{I}] = 0 \tag{10}$$

where $\mathbf{A}(w)$ ($\mathbf{A}(w^*)$) is the L-square matrix with elements $a_{ij} = w_i w_j$ ($a^*_{ij} = w^*_i w^*_j = (1 - w_i)(1 - w_j)$) if $|i - j| = 1$ and zero otherwise, and $\mathbf{I}$ is the unit matrix.

To write the secular equations in this more general form has one advantage, namely it allows us to calculate the first-order correction to $E_1 = 0$ and $E_2 = U$ directly from (9) and (10) for an arbitrary configuration of ions. Now, we see that both determinants in (9) and (10) for any $w = \{w_1, w_2, \ldots, w_L\}$ may be decomposed as

$$D_1^{n_1} D_2^{n_2} \ldots D_i^{n_i} \tag{11}$$

where D_i are determinants of the i-square Jacobi matrices of the form

$$\mathbf{J} = \begin{pmatrix} E & 1 & 0 & \ldots & 0 & 0 \\ 1 & E & 1 & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & E & 1 \\ 0 & 0 & 0 & \ldots & 1 & E \end{pmatrix} \tag{12}$$

and n_i denotes their number. However, the solution of the problem $D_i = 0$ for any $i = 1, 2, \ldots, L$ may be expressed in the closed form as

$$\epsilon(k, i) = -2 \cos[k\pi/(i + 1)] \qquad k = 1, 2, \ldots, i \tag{13}$$

so that the final solution of the secular equations may be obtained at once in terms of $\epsilon_0(k, i)$ and $\epsilon_U(k, i)$, where the subscripts 0 and U are used to denote the first-order corrections to $E_1 = 0$ and $E_2 = U$, respectively (if these are not necessary we omit them). Thus, for any configuration of ions, the total spectrum of the model calculated in the first-order perturbation theory can be expressed as a combination of the spectra $\epsilon(k, i)$, and the ground-state energy corresponding to fixed values N_e and N_i can be found such that we gradually occupy by electrons the low-lying energy levels from $\epsilon(k, i)$. The most important question to ask now is which configuration of ions minimizes the energy $E(N_e, N_i, w)$ if the total electron number and the total ion number are fixed, or in other words which spectrum calculated by using the procedure outlined above leads to the lowest energy of the system. It can be shown [10] that it is a configuration for which the degeneracy of

the energy levels E_1 and E_2 is completely removed, i.e. (see (9), (10)) a configuration with the largest connected cluster of unoccupied sites ($E_1 = 0$) or a configuration with the largest connected cluster of occupied sites ($E_2 = U$). Any division of the largest connected cluster of unoccupied (occupied) sites into two connected clusters mutually separated by occupied (unoccupied) sites increases the energy of the system, and thus the ground-state configuration for $|U| \to \infty$ will be the configuration with the largest connected cluster of unoccupied (occupied) sites—the segregated phase.

4. Finite interaction strength

To analyse some energetic and structural ground-state properties of the Falicov–Kimball model at large, but finite, U we use the second-order degenerate perturbation theory [9]. The scheme consists of diagonalizing the secular matrix with elements

$$V'_{nn'} = V_{nn'} + \sum_m \frac{V_{nm}V_{mn'}}{E_n^{(0)} - E_m^{(0)}} \tag{14}$$

where V refers to a perturbation term, n, n' are labels for umperturbed degenerate ground states, and m labels states not degenerate with the ground states. For the Falicov–Kimball model this scheme leads to the following secular equation:

$$\det(\mathbf{T}' - E\mathbf{I}) = 0, \tag{15}$$

where the matrix elements $T'_{nn'}$ of the N_i- or $(L - N_i)$-square matrix $\mathbf{T}'$ are given by

$$T'_{nn'} = t_{nn'} \pm \frac{1}{U}\sum_m t_{nm}t_{mn'}. \tag{16}$$

If we calculate the second order corrections to the energy level $E_1 = 0$ ($E_2 = U$), then n and n' in (16) denote unoccupied (occupied) sites, whereas m denotes occupied (unoccupied) sites and the correct sign in front of the sum is $-$ (+). Before the proof of some general properties of the one-dimensional Falicov–Kimball model in the limit of strong correlations let us first test the convenience of the above-outlined perturbation procedure for studying the ground-state phase diagram of the model.

In figure 1 we present the phase diagram of the one-dimensional Falicov–Kimball model calculated in the framework of perturbation theory for the segregated configuration and all periodic configurations with $N_i = \frac{1}{2}L$ and periods less than nine: $w_1 = \{10\ldots\}$, $w_2 = \{1100\ldots\}$, $w_3 = \{111000\ldots\}$, $w_4 = \{110100\ldots\}$, $w_5 = \{11110000\ldots\}$, $w_6 = \{11101000\ldots\}$, $w_7 = \{11100100\ldots\}$, $w_8 = \{11011000\ldots\}$, $w_9 = \{11010100\ldots\}$, $w_{10} = \{11010010\ldots\}$. For these periodic configurations the secular equation (15) is enormously simplified and can be immediately solved. Putting electrons into the low-lying energy levels of the new spectra, one can at once find energies corresponding to these configurations. The phase diagram is then determined by comparing the energy of each periodic phase with the energy of the segregated phase and plotting the lowest-energy state as a function of the electron concentration n_e and the interaction strength U. The inset in figure 1 shows the exact phase diagram of the model calculated numerically for the same ion configurations using the method described in [7]. We see that perturbation results reproduce surprisingly well the exact results obtained by Freericks and Falicov, even for relatively

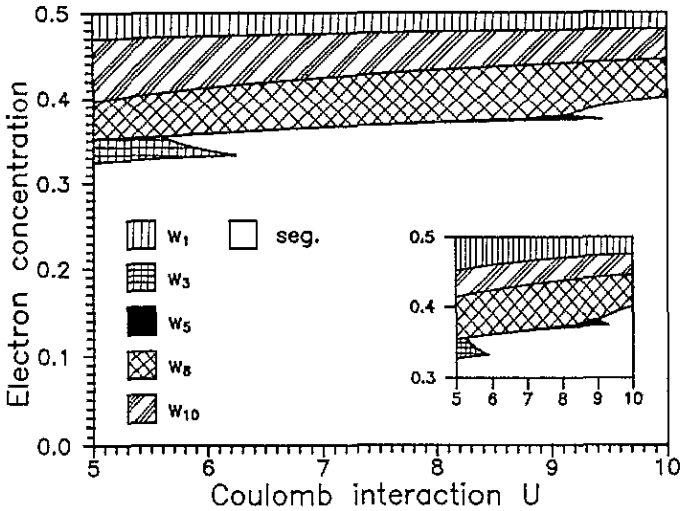

Figure 1. The phase diagram calculated for the segregated configuration and all periodic configurations with $N_i = \frac{1}{2}L$ and periods less than nine. The inset shows the phase diagram calculated exactly using the method described in [7].

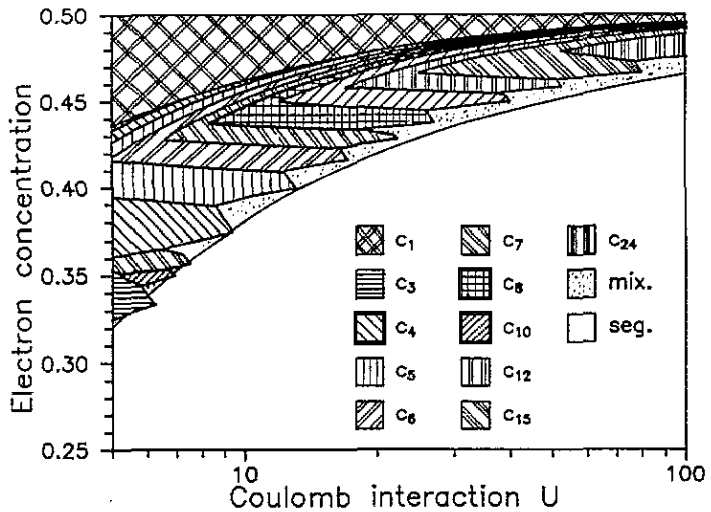

Figure 2. The phase diagram calculated for c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, c_{10}, c_{12}, c_{15}, c_{24}, c_{60}, c_{120}, and the segregated configuration. A domain denoted 'mix'. is a mixture of many small phases.

small values of interaction constant $U \simeq 5$. The fact that perturbation results for $U > 5$ reproduce the exact results very well is obviously due to the theorem of Gerschgorin, which works in these interval and which states that for any ion configuration the electron states are split into two non-overlapping bands: the lower one bounded to $[-2, 2]$, contains exactly $1 - n_i$ states per site, the higher, bounded from below by $U - 2$, contains n_i states per site, which is in agreement with our perturbation results.

Let us now discuss in detail some structural ground-state properties of the model.

Let N_i be arbitrary, then the secular equation (15) for the segregated configuration $w_s = \{11\ldots100\ldots0\}$ takes the form

$$D_N = \begin{vmatrix} \lambda/U - E & -1 & 0 & \ldots & 0 & 0 \\ -1 & -E & -1 & \ldots & 0 & 0 \\ 0 & -1 & -E & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & -E & -1 \\ 0 & 0 & 0 & \ldots & -1 & \lambda/U - E \end{vmatrix} = 0 \tag{17}$$

and it can be directly solved, with the result

$$\epsilon(n, N) = -2\cos[n\pi/(N+1)] + [4\lambda/U(N+1)]\sin^2[n\pi/(N+1)] - \left[2(2N-4)/U^2(N+1)^2\right]\sin^2[n\pi/(N+1)]\cos[n\pi/(N+1)] \tag{18}$$

where $N = L - N_i$, $\lambda = -1$, $n = 1, 2 \ldots L - N_i$ if the second-order corrections to the $(L - N_i)$-fold degenerate energy level $E_1 = 0$ are calculated and $N = N_i$, $\lambda = 1$, $n = 1, 2, \ldots, N_i$ for the N_i-fold degenerate energy level $E_2 = U$. Comparing w_s with w_2, w_3, w_5 one can see that the configurations w_2, w_3, and w_5 are composed of $\frac{1}{4}L$, $\frac{1}{6}L$, and $\frac{1}{8}L$ segregated configurations of lengths 4, 6, and 8, and the length of the connected clusters of occupied sites in these segregated configurations are 2, 3, and 4. Therefore, in the strong-coupling limit the energy spectrum corresponding to w_2, w_3, and w_5 may be directly obtained using the expression (18). Certainly the same is true for other configurations of this kind. In figure 2 we present the phase diagram of the model for the following periodic configurations of this kind: c_1, c_3, c_4, c_5, c_6, c_7, c_8, c_{10}, c_{12}, c_{15}, c_{24}, and the segregated phase. Here we introduce a new general notation $c_i = \{11\ldots100\ldots0\ldots\}$ for the periodic configurations composed of connected clusters of occupied and unoccupied sites of length i; $c_1 = \{10\ldots\}$, $c_2 = \{1100\ldots\}$, etc).

It is seen that all observations made by Freericks and Falicov for periodic phases with $N_i = \frac{1}{2}L$ and periods less than nine still hold: (1) the alternating phase $\{10\ldots\}$ is the ground state at the half-filled band point ($N_e = N_i = \frac{1}{2}L$) for all values of interaction strength; (2) the phase diagrams are enormously simplified as U increases and the segregated phase becomes dominant; and (3) some phases (e.g., c_7, c_{10}) that disappear from the phase diagram as U increases may reappear at larger values of U. Besides the observations of Freericks and Falicov we find that new phases c_5 ,c_6, c_7,... are distributed between the segregated phase w_s and phases w_8 and w_{10}, which are gradually suppressed (see figure 3). Furthermore, for $U > 8$ the largest phase islands of the configurations c_i ($i = 5, 6, \ldots$) are distributed regularly in order of increasing i, and this trend still holds when further periodic configurations with much larger periods are added.

We observed that the configuration $c_{L/4}$ is not the ground state for any value of U and n_e. The configuration $c_{L/4} = \{11\ldots100\ldots011\ldots100\ldots0\}$ may however be obtained such that we divide the segregated phase $w_s = \{11\ldots100\ldots0\}$ into two identical parts. The fact that this configuration is not present in the phase diagram of the model indicated that division of the segregated phase into two identical parts is energetically unfavourable. As was mentioned in the previous section for $|U| \to \infty$ it is energetically unfavourable to divide the large connected cluster of occupied (unoccupied) sites into two connected clusters of occupied (unoccupied) sites separated by unoccupied (occupied) sites and thus the segregated phase was the ground state of the one-dimensional Falicov–Kimball model for all electron concentrations except the specific values $n_e = 1 - n_i$ and $n_e = n_i$. Next

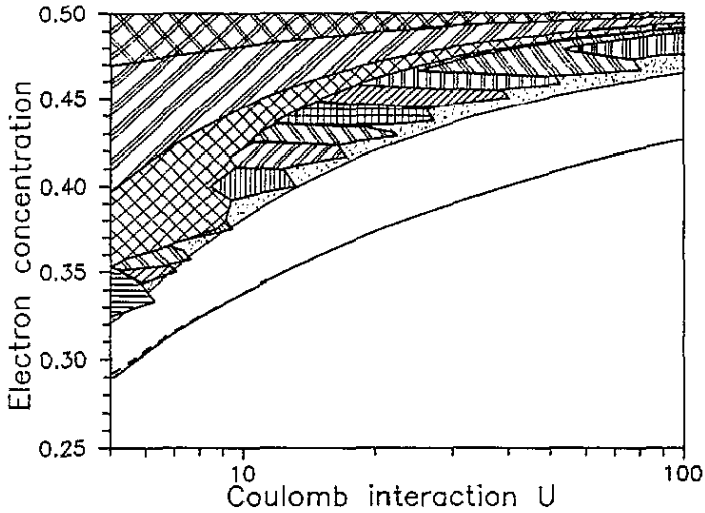

Figure 3. The phase diagram calculated for all configurations from figures 1 and 2. The broken and full curves are lower bounds for the segregated configuration calculated for the transitions $w_S \rightarrow w_{D_2}$ and $w_S \rightarrow w_{D_1}$ respectively.

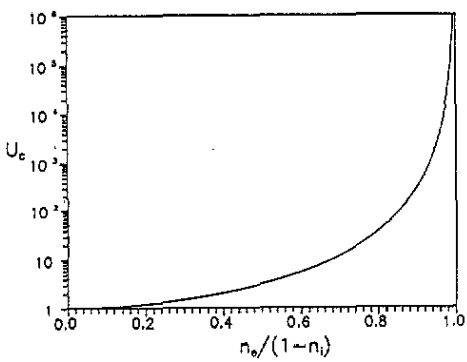

Figure 4. The critical interaction strength U_c as a function of the electron- and ion-density ratio $n_e/(1-n_i)$.

we show that unlike the case $|U| \rightarrow \infty$, for finite U there exists some critical value of the electron concentration n_e above which the segregated phase is unstable, and the large connected cluster of occupied (unoccupied) sites divides into two connected clusters mutually separated by unoccupied (occupied) sites. We give the analytical expression for this boundary.

In the general case when the segregated phase consists of two large connected clusters of occupied and unoccupied sites of length N_i and $L - N_i$, the second-order corrections to the $(L - N_i)$-fold degenerate energy level $E_1 = 0$ are given by (18). Let us now investigate how this energy spectrum (it is sufficient to consider only the case $E_1 = 0$ and $U > 0$, since the other cases can be obtained by the application of the symmetries (7) and (8)) is changed if the connected cluster of unoccupied sites in the segregated configuration is divided into two connected clusters of unoccupied sites of lengths N_1 and N_2 mutually separated by one

or more ions. In the second case the secular equation (15) reduces to

$$\begin{vmatrix} -1/U-E & -1 & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ -1 & -E & \dots & 0 & 0 & 0 & 0 & \dots & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & -E & -1 & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & -1 & -1/U-E & 0 & 0 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & -1/U-E & -1 & \dots & 0 \\ 0 & 0 & \dots & 0 & 0 & -1 & -E & \dots & 0 \\ \vdots & \vdots & & \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & \dots & 0 & 0 & 0 & 0 & \dots & -1/U-E \end{vmatrix} = 0 \tag{19}$$

and may be immediately solved since the corresponding determinant of the type $L - N_i$ can be written as $D_1 D_2$, where determinants D_1 and D_2 of the type N_1 and N_2 have the form of the determinant D_N (see (17)), which has already been examined. Therefore (using the expression (18)), the energy spectrum corresponding to the configuration composed of two connected clusters of unoccupied sites separated by two or more ions is given as a combination of spectra $\epsilon(n, N_1)$ and $\epsilon(n, N_2)$.

Let us denote

$$S\left(m, \frac{\pi}{M+1}\right) = -2\sum_{n=1}^{m} \cos\left(\frac{n\pi}{M+1}\right) = 1 - \frac{\sin\left\{(m+\frac{1}{2})[\pi/(M+1)]\right\}}{\sin[\pi/2(M+1)]} \tag{20}$$

then the energy of m electrons placed in the m low-lying energy levels of the spectrum corresponding to the connected cluster of unoccupied sites of length M can be now written as

$$E(m, M) = -\frac{2m}{U(M+1)} + S\left(m, \frac{\pi}{M+1}\right) + \frac{2M-4}{4U^2(M+1)^2} S\left(m, \frac{\pi}{M+1}\right) - \frac{1}{U(M+1)} \times S\left(m, \frac{2\pi}{M+1}\right) - \frac{2M-4}{4U^2(M+1)^2} S\left(m, \frac{3\pi}{M+1}\right). \tag{21}$$

For N_e electrons (remember that $N_e < L - N_i$) the energy of the segregated configuration w_s with one connected cluster of unoccupied sites of length $L - N_i$ and the energy of a configuration w_{D_2}, which consists of two connected clusters of unoccupied sites of lengths N_1 and N_2 ($N_1 + N_2 = L - N_i$) separated by two or more ions, are thus $E_s(N_e, w_s) = E(N_e, L - N_i)$ and $E_D(N_e, w_{D_2}) = E(n_0, N_1) + E(N_e - n_0, N_2)$ respectively, where n_0 in the ground state with a fixed electron number N_e must be chosen to minimize the ground-state energy $E_D(N_e, w_{D_2})$. It can be obtained by taking the integer part of $(N_e + 1)(N_1 + 1)/(L - N_i + 2)$. Comparing these energies one can straightforwardly show that for any electron concentration n_e there exists a critical value $U = U_c$ of the interaction strength, below which $E_D < E_s$, i.e., for $U < U_c$ the segregated phase is unstable and the transition $w_s \to w_{D_2}$ becomes energetically favourable. A detailed analysis of the inequality $E_D < E_s$ made for any division of the large connected cluster of unoccupied sites into two connected clusters of unoccupied sites of lengths N_1 and N_2 separated by two or more ions shows that the lowest-energy configuration for $U < U_c$ is always the configuration with $N_1 = L - N_i - 1$ and $N_2 = 1$, as it would be expected intuitively.

Now, we are ready to give an analytical expression for the boundary $U_c(N_e)$, below which the segregated phase cannot be the ground state of the one-dimensional Falicov–Kimball model, because the configurations $w_{D_2} = \{00...01...101...1\}$ (where the length of the connected cluster of unoccupied sites is $L - N_i - 1$ and the length of the first connected cluster of occupied sites is at least two) always have lower energy than that corresponding to w_s.

The energy spectrum for $\epsilon(n, w_{D_2})$ is given as the combination of spectrum (18) with $N = L - N_i - 1$ and the single energy level $-2/U$, therefore

$$E_D(N_e, w_{D_2}) = \begin{cases} E(N_e, L - N_i - 1) & \text{for } N_e \leqslant p_0 \\ E(N_e - 1, L - N_i - 1) - 2/U & \text{for } N_e > p_0. \end{cases} \tag{22}$$

Here p_0 is the integer part of

$$q = \left[(L - N_i)/\pi\right] \cos^{-1}\left\{\tfrac{1}{4}U(L - N_i) - \sqrt{[\tfrac{1}{4}U(L - N_i)]^2 - \tfrac{1}{2}(L - N_i - 2)}\right\} \tag{23}$$

which is defined by the condition

$$\epsilon(q, L - N_i - 1) = -2/U. \tag{24}$$

Comparing (22) with the energy of the segregated phase $E_s(N_e, w_s)$ we obtain the analytic expression for the boundary $U_c(N_e)$, below which the segregated phase cannot be the ground state of the one-dimensional Falicov–Kimball model

$$U_c = \left(b - \sqrt{b^2 - ac}\right)/2a \tag{25}$$

where

$$a = S\left[N_e, \pi/(N+1)\right] - S\left(N_e - 1, \pi/N\right) \qquad (N = L - N_i)$$

$$b = [1/(N+1)]\left[2N_e + S\left[N_e, 2\pi/(N+1)\right]\right\} - (1/N)\left[2(N_e - 1) + S\left(N_e - 1, 2\pi/N\right)\right] - 2$$

$$c = \left\{S\left[N_e, \pi/(N+1)\right] - S\left[(N_e, 3\pi/(N+1)\right]\right\}(2N-4)/(N+1)^2 - \left[S\left(N_e - 1, \pi/N\right)\right.$$
$$\left. - S\left(N_e - 1, 3\pi/N\right)\right](2N-6)/N^2.$$

The critical interaction strength U_c as a function of the electron- and ion-density ratio $n_e/(1 - n_i)$ is plotted in figure 4. We see that even for considerably large deviations from the singular point $n_e/(1 - n_i) = 1$, the values U_c are extremely large, which is in agreement with results of Brandt [8]. On the other hand, it should be mentioned that our estimate of the lower bound $U^- \equiv U_c$, below which the segregated phase cannot be the ground state of the model, is better than the estimate of Brandt, who investigated the stability of the segregated phase with respect to 'evaporation'. However, his estimate of the upper bound U^+, above which only the segregated phase is the ground state of the model, is quite good for $n_e/(1 - n_i) > 0.5$ and it together with our results for U_c yields sharp bounds for the segregated state. Of course, since our results were obtained in the strong-interaction limit using perturbation theory, it is necessary to bound the phase diagram from below with some physically reasonable value of the interaction strength U_0, above which the perturbation procedure gives reasonable results. Tests, we made (see figure 1) show that this value should be relative small ($U_0 \simeq 5$).

The critical value U_c was obtained for the case when a single unoccupied site and the connected cluster of unoccupied sites of length $L - N_i - 1$ were separated by $N_i \geqslant 2$ ions. Repeating the previous analysis for the case $N_i = 1$ one can show with some more effort that the energy spectrum corresponding to this configuration w_{D_1} is given as

$$\epsilon(n, w_{D_1}) = \epsilon(n, w_{D_2}) - \left[1/U^2(L - N_i)\right] \sin^2\left[n\pi/(L - N_i)\right] / \cos\left[n\pi/(L - N_i)\right]$$

for $n = 1, 2, \ldots, L - N_i - 1$ and

$$\epsilon(n = L - N_i, w_{D_1}) = -2/U.$$

Thus the ground state corresponding to w_{D_1} has for any electron number N_e lower energy than the ground state corresponding to w_{D_2} as one would expect.

If these configuration are taken into account, then the area of stability of the segregated phase is considerably reduced in the ground state phase diagram (see figure 3) but it is still large enough. Let us note that in the domain where the segregated configuration is stable, the U dependence of the ground state energy (which follows from (18)) has qualitatively the same form as the exact U dependence of the one-dimensional Hubbard model in the limit of strong interactions [11]. The total U dependence of the one-dimensional Falicov–Kimball model calculated for the phase diagram from figure 3 is shown in figure 5.

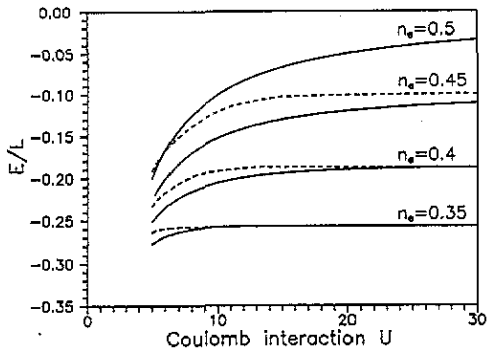

Figure 5. The U dependence of the ground-state energy of the one-dimensional Falicov–Kimball model calculated for the phase diagram shown in figure 3 (broken curves) and for incoherent mixtures of the segregated and period-two phases (full curves).

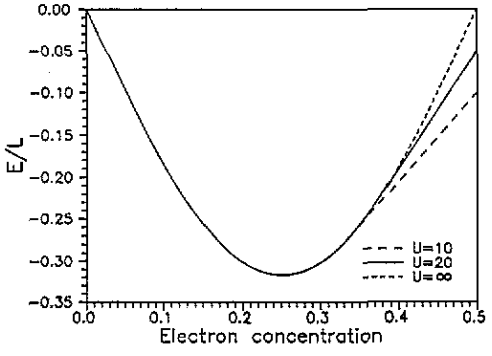

Figure 6. The ground-state energy of the one-dimensional Falicov–Kimball model calculated for incoherent mixtures of the segregated and period-two phases as a function of n_e

It was shown above that for finite U there exists some critical value of the electron concentration above which the segregated configuration w_s cannot be the ground state of the model, because there the configuration w_{D_1} always has lower energy than w_s. One can ask what happens for w_{D_1} for higher band fillings and there are ways to generalize our previous ideas. For fixed $N_i = \frac{1}{2}L$ we examined all possible incoherent mixtures $w^{\text{incoh}}(N)$ of the segregated configuration of length N and the alternating configuration of length $L-N$. In agreement with (25) we have found that $w^{\text{incoh}}(L) \equiv w_s$ is the ground state of the model for $U > U_c \equiv U_L$, and below U_c some incoherent mixture with $N \neq L$ becomes stable. In particular, $w^{\text{incoh}}(N)$ $(N < L)$ is stable in the narrow domain bounded by U_N and U_{N-1}, where U_N and U_{N-1} can be obtained directly from the conditions $E[N_e, w^{\text{incoh}}(N)] =$

$E[N_e, w^{incoh}(N-1)]$ and $E[N_e, w^{incoh}(N-1)] = E[N_e, w^{incoh}(N-2)]$. Furthermore we found that neither periodic configuration from the phase diagram shown in figure 3, excluding the alternating phase can be the ground state of the model if these incoherent mixtures are taken into account, and the alternating phase will be the ground state only for $N_e = \frac{1}{2}L$. To investigate whether the ground state corresponding to w^{incoh} is conducting or insulating, we compute the quantity $\Delta\mu = E(N_e+1, N_i) + E(N_e-1, N_i) - 2E(N_e, N_i)$. (The N_e dependence of the ground-state energy calculated for these incoherent mixtures is plotted in figure 6 for three different interaction strengths.) Using the criterion of Kennedy and Lieb [3], which states that there is a gap of the second kind at N_e, N_i if $\Delta\mu \geqslant \epsilon > 0$, with ϵ being independent of the size of the system, we arrived at the conclusion that for all $N_e < \frac{1}{2}L$ the ground state is conducting.

Finally let us briefly discuss the model for $n_i \to 0$ ($n_i \to 1$). For $N_i = 2$ we found that from among all possible distributions of N_i ions and $L - N_i$ unoccupied sites, the segregated configuration is the ground state for $U > U_c$, where U_c is given by (25). If $U < U_c$ the configuration $\{10100\ldots0\}$ is stable. Analogously for all possible distributions of three ions and $L-3$ unoccupied sites we found that the segregated phase is stable if $U > U_{c_1}$. In the domain $U_{c_2} < U < U_{c_1}$ the configuration $w = \{110100\ldots0\}$ is the ground state and for $U < U_{c_2}$ the configuration $w' = \{1010100\ldots0\}$ is stable. Here U_{c_1} is given by (25) and U_{c_2} can be obtained from the condition $E(N_e, w) = E(N_e, w')$.

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