GROUND STATE PROPERTIES OF THE FALICOV-KIMBALL MODEL IN THE STRONG COUPLING LIMIT

PAVOL FARKASOVSKÝ, IVAN BAŤKO
Institute of Experimental Physics, Slovak Acad. Sci., Watsonova 47, 043 53 Košice, Slovak Republic

Received 16 December 1992

We present some analytic results concerning the ground state of the one-dimensional Falicov-Kimball model in the strong coupling limit. Using the perturbation theory, we find: (i) The well-expected phase segregation takes place for \( |U| \to \infty \) (\( U \) is the interaction strength). (ii) For finite \( U \) there exists the critical value of the interaction strength \( U = U_c \), below which the segregated phase — an incoherent mixture of the empty and full lattices cannot be the ground state of the model. We give the analytical expression for this boundary. Finally, we discuss the phase diagram of the model for some special configuration of ions.

1. Introduction

Much effort is presently spent to understand the correlation effects induced by strong, short-ranged interactions in Fermi systems. The motivation is clearly due to discoveries of new materials like the heavy-fermion compounds or the high-temperature superconductors, to mention only these. 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

\[
H = \sum_{ij} t_{ij} c_i^+ c_j + U \sum_i w_i c_i^+ c_i,
\]

where \( c_i^+ (c_i) \) are fermionic creation (annihilation) operators for the spinless electron at the 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 by an ion.

The kinetic energy (the first term of (1.1)) 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 \( t_{ij} \). For the conventional Falicov-Kimball model it is usually assumed that \( t_{ij} = -t \) if \( i \) and \( j \) are the nearest neighbors and \( t_{ij} = 0 \) otherwise. The second term represents an on-site interaction between electrons and ions that can be repulsive \( (U > 0) \) or attractive \( (U < 0) \). In this model
both the total electron number $N_e$ and the total ion number $N_i$ defined by

$$N_e = \sum_i c_i^+ c_i, \quad N_i = \sum_i w_i$$

(1.2)

are conserved quantities.

The Falicov-Kimball model was originally introduced to study mixed-valence states in rare-earth compounds [1]. There the moving particles play the role of band s electrons and the 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 (1.1) 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 s and ions, where the following ion configurations: the checkerboard configuration, the completely empty and fully occupied configurations may be ground states. (3) Kennedy and Lieb [3] proved that the ground state has a 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 there does not exist the exact solution of the model for $d = 1$ dimension). They presented the coherent and incoherent phase diagrams calculated numerically for the segregated phase and all periodic phases with periods less than 9 and $N_i = L/2, L/3$, where $L$ is the number of lattice sites. On the base of these results they formulated the conjecture, the so-called segregation principle, which states the following: In the limit $|U/t| \rightarrow \infty$ the segregated phase, which is an incoherent mixture of the empty and full lattices with the 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 $(U/t) \rightarrow \infty$ and $n_e = n_i$ for $(U/t) \rightarrow -\infty$ ($n_e = N_e/L, n_i = N_i/L$). (6) Brandt [8] was the first who analytically proved 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. We recover some results already obtained by Freericks and Falicov [7] and Brandt [8] (e.g., the phase segregation at large $U$) and furthermore we present some new exact 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, etc.).

2. Some properties of the model

Before the performance of the perturbative analysis let us recall some general properties of the Hamiltonian (1.1). For a given ion configuration \( w = \{w_1, w_2, \ldots, w_L\} \), on the one-dimensional lattice of \( L \) sites, the Hamiltonian (1.1) is the second quantized version of the single particle Hamiltonian

\[
\mathbf{h}(w) = \mathbf{T} + U \mathbf{W},
\]

where \( \mathbf{T} \) is the \( L \)-square matrix with elements \( t_{ij} = -t \) if \( i, j \) are the nearest neighbors and \( t_{ij} = 0 \) otherwise, and \( \mathbf{W} \) is the \( L \)-square diagonal matrix with elements \( w_i \). In spite of its form the considered model is not one of the 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

\[
E_G(U, N_e, N_i) = \min\{E(U, N_e, w)| \sum_i w_i = N_i\},
\]

where \( E(U, N_e, w) \) is the ground state energy for the 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

\[
E(U, N_e, w^*) = E(-U, N_e, w) + UN_e, \quad w^* = \{1 - w_1, 1 - w_2 \ldots 1 - w_L\}
\]

and

\[
E(U, N_e, w) = E(-U, N - N_e, w) + UN_i,
\]

which enable to reduce the necessary parameter space as follows: \( N_e \leq L/2 \) and \( N_i \leq L/2 \). Therefore, we can restrict ourselves only to these cases, the remaining cases may be deduced from a combination of the above mentioned symmetries.

3. Perturbative analysis, infinite \( U \)

To show some characteristic features and to define the basic conceptions 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 (1.1) 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].
straightforward procedure for $E_1 = 0$ and $E_2 = U$ leads to the following secular equations

$$\begin{pmatrix}
E & w_1^* w_2^* & 0 & \ldots & 0 & 0 \\
w_1^* w_2^* & E & w_2^* w_3^* & \ldots & 0 & 0 \\
0 & w_2^* w_3^* & E & \ldots & 0 & 0 \\
& \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & E & \omega_{L-1}^* \omega_L^* \\
0 & 0 & 0 & \ldots & w_{L-1}^* \omega_L^* & E \\
\end{pmatrix} = 0, \quad (3.1)$$

and

$$\begin{pmatrix}
E & w_1 w_2 & 0 & \ldots & 0 & 0 \\
w_1 w_2 & E & w_2 w_3 & \ldots & 0 & 0 \\
0 & w_2 w_3 & E & \ldots & 0 & 0 \\
& \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & E & \omega_{L-1} \omega_L \\
0 & 0 & 0 & \ldots & w_{L-1} \omega_L & E \\
\end{pmatrix} = 0, \quad (3.2)$$

where the conjugate variables $w_i^*$ are defined by interchanging occupied and unoccupied sites, i.e., $w_i^* = 1 - w_i$. To write the secular equations in this more general form has one advantage, namely, it allows to calculate the first order correction to $E_1 = 0$ and $E_2 = U$ directly from (3.1) and (3.2) for arbitrary configuration of ions. Now, we see that both determinants in (3.1) and (3.2) for any $w = \{w_1, w_2, \ldots, w_L\}$ may be decomposed as

$$D_1 \cdot D_2 \cdot \ldots \cdot D_n,$$

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

$$J = \begin{pmatrix}
E & 1 & \ldots & 0 & 0 \\
1 & E & \ldots & 0 & 0 \\
& \vdots & \ddots & \vdots & \vdots \\
0 & 0 & \ldots & 1 & E \\
\end{pmatrix} \quad (3.4)$$

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

$$\epsilon(k, i) = -2 \cos \left( \frac{k \pi}{i+1} \right), \quad k = 1, 2, \ldots, i, \quad (3.5)$$

so that the final solution of the secular equations may be at once obtained in terms of $\epsilon_0(k, i)$ and $\epsilon_U(k, i)$, where the subscript 0 and $U$ is used to denote the first
order correction to $E_1 = 0$ and $E_2 = U$, respectively (if it is 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 $\varepsilon(k, i)$ 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-laying energy levels from $\varepsilon(k, i)$.

Now the most important question is to ask which configuration of ions minimize 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.

To give the answer to this question, let us consider two different configurations of ions $w$ and $\tilde{w}$. Let $w$ be a configuration for which the degeneracy of the energy levels $E_1$ or $E_2$ is completely removed. As follows from (3.1)–(3.2) for fixed $N_i$, it will be a configuration with the largest connected cluster of unoccupied sites ($E_1 = 0$) or a configuration with the largest connected cluster of occupied sites ($E_2 = U$). Next we show that any division of the largest connected cluster of unoccupied (occupied) sites into two connected clusters mutually separated by occupied (unoccupied) sites (configuration $\tilde{w}$) increases the energy of the system, so that the transition $w \rightarrow \tilde{w}$ is unfavorable and thus the ground state configuration will be $w$, i.e., the segregated phase.

Let $N$ and $N_1, N_2$ be the length of connected clusters of unoccupied (occupied) sites in $w$ and $\tilde{w}$. Then the spectrum for $w$ is given by $\varepsilon(k, N)$ and the spectrum for $w$ is given as a combination of the spectra $\varepsilon(k, N_1)$ and $\varepsilon(k, N_2)$.

Putting electrons on the low-laying energy levels of these spectra, one can at once find energies corresponding to $w$ and $\tilde{w}$ ($N = N_1 + N_2$):

$$E(N_e, N, w) = S \left( N_e, \frac{\pi}{N + 1} \right),$$

$$E(N_e, N_1, n_0, \tilde{w}) \equiv E(N_1) = S \left( n_0, \frac{\pi}{N_1 + 1} \right) + S \left( N_e - n_0, \frac{\pi}{N - N_1 + 1} \right),$$

where

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

and $n_0$, in the ground state with a fixed electron number $N_e$, must be chosen to minimize the ground state energy $E(N_e, \tilde{w})$. Straightforward calculations show that $n_0$ can be obtained by taking the integer part of $q = (N_e + 1)(N_1 + 1)/(N + 2)$. The function $E(x)$ given by (3.7) is schematically shown in Fig. 1. It has $N_e$ maxima localized at

$$x_{\max}(k) = \frac{(N + 2)k}{N_e + 1} - 1, \quad k = 1, 2, \ldots N_e$$

and $N_e - 1$ minima localized at

$$x_{\min}(k) = \frac{(N + 2)k + N/2 - N_e}{N_e + 1}, \quad k = 1, 2, \ldots N_e - 1,$$
Fig. 1. Schematic plot of the function $E(x)$ given by (3.7). The function plotted as $E^+ \equiv E(N_e, N_1, q, \tilde{w})$ is the upper bound of $E(N_1)$ and the function plotted as $E^- \equiv E(N_e, N_1, q - \frac{1}{2}, \tilde{w})$ is the lower bound of $E(N_1)$.

but the total minimum it reaches at $x = 0$ and $x = N$ as it is expected.

Remark. Since there are only two $(L - N_i)$ and $N_i$-fold degenerate energy levels $E_1 = 0$ and $E_2 = U$, the second order correction goes at least as $1/U$ and vanishes for $|U| \to \infty$.

Thus, we see that the ground state configuration of the one-dimensional Falicov-Kimball model in the limit $U \to \infty$ is the configuration which completely removes the degeneracy of the $(L - N_i)$-fold degenerate energy level $E_1 = 0$, i.e., the configuration with the largest connected cluster of unoccupied sites for fixed $N_i$ $(N_e < L - N_i)$, or the configuration which completely removes the degeneracy of the $N_i$-fold degenerate energy level $E_2 = U$, i.e., the configuration with the largest connected cluster of occupied sites $(L - N_i < N_e)$. Of course, in consequence of a validity of periodic boundary conditions both configurations are equivalent, so that we may conclude that for $U \to \infty$ the segregated phase is the ground state for all values of the electron concentration except the specific value $n_e = 1 - n_i$. The case $U < 0$ can be considered in the similar manner. The lower energy level is now $E_2 = U$, which is $N_i$-fold degenerate and thus the segregated phase will be the ground state for all values of the electron concentration except the value $n_e = n_i$. At the points $N_e = N_i$ and $N_e = L - N_i$ the ground state energy is degenerate up to the first order, so that higher order corrections of the perturbation theory must be included to find a ground state configuration.

4. Finite interaction strength

In this section we investigate ground state properties of the one-dimensional Falicov-Kimball model for finite interaction strength $U$. We still assume that $U \gg 1$ (this condition will be specified later) and we calculate the higher order corrections
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to the degenerate energy levels $E_1 = 0$ and $E_2 = U$ using the standard perturbation theory [9]. For the Falicov-Kimball model this theory leads to the following secular equation

$$\det(T' - EI) = 0,$$  

(4.1)

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

$$T'_{ij} = t_{ij} \pm \frac{1}{U} \sum_m t_{im} t_{mj}.$$  

(4.2)

If we calculate the second order corrections to the energy level $E_1 = 0$ ($E_2 = U$), then $i$ and $j$ in (4.2) denote unoccupied (occupied) sites, whereas $m$ denotes occupied (unoccupied) sites and the correct sign in front of the sum is $- (+)$. Before proving 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 to study the ground state phase diagram of the model.

Let $w_1, w_3, w_4, w_{L/2}$ be the periodic configuration with period two, six, eight, $L$ (see below) and let $w_8$ and $w_{10}$ be the periodic configuration 8 and 10 from Ref. 7. For $U > 5$ the mentioned configurations are just ground state configurations from among all periodic phases with $N_i = L/2$ and periods less than 9 as it was shown by Freericks and Falicov [7].

The secular equation (4.1) for the alternating phase $w_1 = \{1010\ldots10\}$ takes the form

$$\begin{vmatrix}
-2/U - E & -1/U & 0 & \ldots & 0 & -1/U \\
-1/U & -2/U - E & 0 & \ldots & 0 & 0 \\
0 & -1/U & -2/U - E & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & -2/U - E & -1/U \\
-1/U & 0 & 0 & \ldots & -1/U & -2/U - E \\
\end{vmatrix} = 0 \quad (4.3)$$

and may be immediately solved with the result

$$\varepsilon(k_n) = -\frac{4}{U} \cos^2(k_n/2), \quad k_n = \frac{2\pi n}{N_i}, \quad n = 0, 1, 2, \ldots, N_i - 1. \quad (4.4)$$

For periodic configurations the secular equation (4.1) is enormously simplified. Particularly, for considered special configurations $w_3, w_4, w_8$, and $w_{10}$ (4.1) is reduced to

$$\begin{vmatrix}
E + 1/U & 1 & 0 \\
1 & E & 1 \\
0 & 1 & E + 1/U \\
\end{vmatrix}^{L/6} = 0 \quad \text{for } w_3 = \{111000\ldots\}, \quad (4.5)$$

Solving these equations, we obtain the following second order corrections to $L - N_i = L/2$-fold degenerate energy level $E_1 = 0$ (corresponding corrections to $L/2$-fold degenerate energy level $E_2 = U$ may be obtained in the same way).

$w_3 = \{110000\ldots\}$

\begin{align*}
\epsilon_1 &= \frac{1}{2} \left( \sqrt{x^2 + 8 + x} \right) \approx -\sqrt{2} - \frac{x^2}{2} - \frac{\sqrt{2}}{16} x^2 + O(x^3), \\
\epsilon_2 &= -1/U, \\
\epsilon_3 &= \frac{1}{2} \left( \sqrt{x^2 + 8 - x} \right) \approx \sqrt{2} - \frac{x^2}{2} + \frac{\sqrt{2}}{16} x^2 + O(x^3),
\end{align*}

where $x = 1/U$ and each energy level $\epsilon_1, \epsilon_2$ and $\epsilon_3$ is $(L/6)$-fold degenerate.

$w_4 = \{11110000\ldots\}$

\begin{align*}
\epsilon_1 &= -\frac{1}{2} \sqrt{x^2 - 2x + 5} + x + 1 \approx -\frac{\lambda^+}{2} + \frac{\alpha^{-}}{10} x + \frac{\lambda^{+} \alpha^{-}}{100} x^2 + O(x^3), \\
\epsilon_2 &= -\frac{1}{2} \sqrt{x^2 + 2x + 5} + x - 1 \approx -\frac{\lambda^{-}}{2} - \frac{\alpha^{+}}{10} x - \frac{\lambda^{-} \alpha^{+}}{100} x^2 + O(x^3), \\
\epsilon_3 &= \frac{1}{2} \sqrt{x^2 - 2x + 5} - x - 1 \approx \frac{\lambda^{-}}{2} - \frac{\alpha^{+}}{10} x - \frac{\lambda^{-} \alpha^{+}}{100} x^2 + O(x^3), \\
\epsilon_4 &= +\frac{1}{2} \sqrt{x^2 + 2x + 5} - x + 1 \approx \frac{\lambda^{+}}{2} + \frac{\alpha^{-}}{10} x + \frac{\lambda^{+} \alpha^{-}}{100} x^2 + O(x^3),
\end{align*}

where $\lambda^\pm = \sqrt{5} \pm 1$ and $\alpha^\pm = \sqrt{5} \pm 5$.

$w_{10} = \{11010010\ldots\}$
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\[
\begin{align*}
\epsilon_1 &= -\frac{1}{2}\sqrt{5x^2 - 2x + 1} + 3x + 1, \\
\epsilon_2 &= -\frac{1}{2}\sqrt{5x^2 + 2x + 1} + 3x - 1, \\
\epsilon_3 &= \frac{1}{2}\sqrt{5x^2 - 2x + 1} - 3x + 1, \\
\epsilon_4 &= \frac{1}{2}\sqrt{5x^2 + 2x + 1} - 3x + 1,
\end{align*}
\tag{4.11}
\]

Comparing (4.5) and (4.7), we see that the energy spectrum corresponding to \(w_8\) consists of three \((L/8)\)-fold degenerate energy levels \(\epsilon_1, \epsilon_2, \epsilon_3\) (given by (4.9)) and the energy level \(\epsilon_4 = -2/U\), which is \((L/8)\)-fold degenerate too. Finally, let us solve the secular equation for the segregated phase \(w_8 = \{11011000\ldots\}\). Unlike the previous cases, which were studied for \(N_1 = L/2\), now we examine the general case when the number of occupied sites is \(N_1\) and the number of unoccupied sites is \(L - N_1 = N\). The secular equation for the segregated configuration \(w_8\) has the form (the case \(E_1 = 0\) is considered)

\[
D_N = \begin{bmatrix}
-1/U - E & -1 & 0 & \ldots & 0 & 0 \\
-1 & -E & -1 & \ldots & 0 & 0 \\
0 & -1 & -E & \ldots & 0 & 0 \\
\vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\
0 & 0 & 0 & \ldots & -E & -1 \\
0 & 0 & 0 & \ldots & -1 & -1/U - E
\end{bmatrix} = 0. \tag{4.12}
\]

It is more difficult to solve this equation for arbitrary \(U\), yet it may be resolved in the strong interaction limit, and it yields for the segregated configuration \(w_8\) the following energy spectrum

\[
\epsilon_0(n, N) = -2\cos\left(\frac{n\pi}{N + 1}\right) - \frac{4}{U(N + 1)} \sin^2\left(\frac{n\pi}{N + 1}\right), \quad n = 1, 2, \ldots, N. \tag{4.13}
\]

Here the subscript 0 denotes that the spectrum corresponds to \(N\)-fold degenerate energy level \(E_1 = 0\), whose degeneracy was completely removed. The energy level \(E_2 = U\) is for the segregated configuration \(w_8\) completely removed too and thus the new spectrum is given by

\[
\epsilon_U(n, N_1) = -2\cos\left(\frac{n\pi}{N_1 + 1}\right) + \frac{4}{U(N_1 + 1)} \sin^2\left(\frac{n\pi}{N_1 + 1}\right), \quad n = 1, 2, \ldots, N_1. \tag{4.14}
\]

Comparing (4.5) and (4.6) with (4.12), one can say that the configuration \(w_3\) (\(w_4\)) is composed of \(L/6\) (\(L/8\)) segregated configurations, whose length is 6 (8) and the length of the connected clusters of occupied sites in these segregated configurations is 3 (4). Therefore the energy spectrum (4.9) and (4.10) may be directly compared with (4.13) and (4.14). Using Taylor series expansion (see (4.9) and (4.10)), we find out that (4.13) and (4.14) yield correct energy spectra up to the order \(1/U\).
Corrections of a higher order may be included too. For example, straightforward application of the perturbation theory to (4.12) gives the following $(1/U^2)$ correction to the energy level $\varepsilon_n$

$$
- \frac{1}{U^2} \left( \frac{2}{N+1} \right)^2 \sum_{m \neq n} \frac{\sin^2 k_n \sin^2 k_m [1 + (-1)^{n+m}]}{\cos k_n - \cos k_m},
$$

which is in agreement with results obtained for special configurations $w_3$ and $w_4$. Because in this paper we investigate the strong interaction limit of the Falicov-Kimball model, then in many considerations it is sufficient to work directly with expressions (4.13) and (4.14).

5. Zero-temperature phase diagram

Now we are ready to construct the phase diagram of the one-dimensional Falicov-Kimball model for the above analysed configurations $w_1, w_3, w_4, w_8, w_{10}, w_s$ and to test the convenience of the outlined perturbation procedure to study the ground state phase diagram of the model. The phase diagram is determined by comparing the energy of each periodic phase $w_1, w_3, w_4, w_8, w_{10}$ 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 $U$. Our results are summarized in Fig. 2. We see that the perturbation results reproduce the exact results obtained by Freericks and Falicov [7] surprisingly well, even for relatively small values of the interaction constant $U \approx 5$. The fact that the perturbation results for $U > 5$ reproduce the exact results very well is obviously due to the theorem of Gerschgorin, which works in this interval and whose 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. Using the same procedure, one can directly show that the phase diagram is unchanged if the remaining configurations from Ref. 7 are added and thus the above considered configurations are really the ground state configurations.

Having the analytic solution for the energy spectrum of the segregated phase with the arbitrary length of occupied (unoccupied) sites, we can immediately investigate a phase diagram of the one-dimensional Falicov-Kimball model for various periodic and aperiodic combinations of these segregated configurations. Although this subject is the contents of our next paper, let us briefly discuss the phase diagram of the model calculated for several such configurations. The modified phase diagram calculated for the following periodic configurations: $c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, w_8, w_{10}$ and the segregated phase are shown in Fig. 3. (Here we introduce a new general notation $c_i = \{ 11...100...0... \}$ for the periodic configurations composed of connected clusters of occupied and unoccupied sites of the length $i$; $c_1 = \{10...\}, c_2 = \{1100...\}, c_3 = \{111000...\}, etc$).

![Diagram](image)

**Fig. 3.** The phase diagram calculated for the periodic configurations $c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, w_8, w_{10}$ and the segregated phase.

It is seen that all observations made by Freericks and Falicov for periodic phases with $N_i = L/2$ and periods less than 9 still hold. (1) The alternating phase $\{10...\}$ is the ground state at the half-filled band point ($N_e = N_i = L/2$) for all values of interaction strength. (2) The phase diagram is enormously simplified as $U$ increases and the segregated phase becomes dominant. (3) Some phases (e.g., $c_7$) that disappear from the phase diagram as $U$ increases may reappear at larger values of $U$. (4) The configuration $c_2$ is not for $U > 5$ the ground state for any value of $n_e$. It should be mentioned that our method unlike that of Freericks and Falicov is applicable to aperiodic configurations too. For example, as it follows from (4.1) the same energy as the configuration $c_4 = \{11110000...\}$ has (for $N_e < L-N_i$) the following aperiodic configuration $c_\alpha = \{110001111110000...11110000\}$ and many other aperiodic configurations too. Besides the observations of Freericks and Falicov we find out that new phases $c_5, c_6, c_7, c_8$ are distributed between the segregated
phase $w_8$ and phases $w_9$ and $w_{10}$, which are gradually suppressed (see Fig. 4). Furthermore, for $U > 8$ the largest phase islands of the configurations $c_i$ ($i = 5, 6, 7, 8$)

![Graph of Coulomb interaction vs. electron concentration](image)

**Fig. 4.** The complete phase diagram calculated for the periodic configurations $c_1, c_2, c_3, c_4, c_5, c_6, c_7, c_8, w_8, w_{10}$ and the segregated phase. The dashed line corresponds to the critical electron concentration $n^*_e$ (see the text below).

are distributed regularly in the order of increasing $i$ and this trend still holds when further configurations with $i > 8$ 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 $c_{L/4} = \{11...100...011...100...0\}$, however, may be obtained such that we divide the segregated phase $w_s = \{11...100...0\}$ into two same parts. The fact that this configuration is not present in the phase diagram of the model indicates that the division of the segregated phase into two same parts is energetically unfavorable. In the previous section we proved that for $|U| \to \infty$ it is energetically unfavorable 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 concentration except the specific value $n_e = 1 - n_i$ and $n_e = n_i$. Next we show that unlike the case $|U| \to \infty$, for finite $U$ 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 is divided into two connected clusters mutually separated by unoccupied (occupied) sites. We give the analytical expression for this boundary.

6. **Phase segregation**

In the general case when the segregated phase consists of two large connected clusters of occupied and unoccupied sites of the lengths $N_i$ and $L - N_i = N$, the energy spectrum corresponding to this configuration (up to the $1/U$ order) is given by (4.13) and (4.14) (to avoid technical difficulties, we do not consider the term of
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order \((1/U^2)\) given by (4.15)).

Let us now investigate how this energy spectrum is changed if the connected cluster of unoccupied sites in the segregated configuration is divided into two connected clusters of unoccupied sites of the length \(N_1\) and \(N_2\) mutually separated by one or more ions. In the second case the secular equation for \(E_1 = 0\) (the case \(E_2 = U\) may be considered analogously) has the form

\[
\begin{pmatrix}
-1/U - E & -1 & \ldots & 0 & 0 & 0 & \ldots & 0 \\
-1 & -E & \ldots & 0 & 0 & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & -1 - E & -1 & 0 & \ldots & 0 \\
0 & 0 & \ldots & 0 & -1 - U - E & 0 & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\
0 & 0 & \ldots & 0 & 0 & 0 & \ldots & -1/U - E \\
\end{pmatrix} = 0,
\]

and may be immediately solved since the corresponding determinant of the type \(N\) 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 4.12)), which was already examined. Therefore the energy spectrum corresponding to the configuration composed of two connected clusters of unoccupied sites separated by two or more ions is given as the combination of spectra \(\varepsilon_0(n, N_1)\) and \(\varepsilon_0(n, N_2)\), where \(N_1\) and \(N_2\) are the lengths of connected clusters of unoccupied sites.

Using the expression (3.8), the energy of \(m\) electrons placed on the \(m\) low-laying energy levels of the spectra corresponding to the connected cluster of unoccupied sites of the length \(M\) can be now written as

\[
E(n, M) = -\frac{2m}{U(M+1)} + S(m, \frac{\pi}{M+1}) - \frac{1}{U(M+1)} S\left(m, \frac{2\pi}{M+1}\right).
\] (6.1)

For \(N_e\) electrons \((N_e < L - N_1)\) then the energy of the segregated configuration \(w_S\) with one connected cluster of unoccupied sites of the length \(N\) and the energy of a configuration \(w_D\), which consists of two connected clusters of unoccupied sites of the lengths \(N_1\) and \(N_2\) \((N_1 + N_2 = N)\) separated by two or more ions is \(E_S(N_e, w_S) = E(N_e, \pi/(N + 1))\), respectively, \(E_D(N_e, w_D) = E(n_0, \pi/(N_1 + 1)) + E(N_e - n_0, \pi/(N - N_1 + 1))\), where \(n_0\) is still calculated by taking the integer part of \((N_e + 1)(N_1 + 1)/(N + 2)\). Comparing this energy, one can straightforwardly show that for any electron concentration \(n_e\) there exists the critical value of the interaction strength \(U = U_c\), below which \(E_D < E_S\), i.e., for \(U < U_c\) the segregated phase is unstable and the transition \(w_S \rightarrow w_D\) becomes energetically favorable. 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

the 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 $N_1 = N - 1$ and $N_2 = 1$, as it should be expected.

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 $w_D = \{00...01...011...1\}$ (where the length of the connected cluster of unoccupied sites is $N - 1$ and the length of the first connected cluster of occupied sites is at least two) have always the lower energy than the one corresponding to $w_S$.

The energy spectrum for $w_D$ is given as a combination of the spectrum (4.13) with $N_1 = N - 1$ and the single energy level $-(2/U)$ and thus

$$E(N_e, w_D) = \begin{cases} \frac{2N_e}{UN} + S \left( N_e, \frac{\pi}{N} \right) - \frac{1}{UN} S \left( N_e, \frac{2\pi}{N} \right) & \text{for } N_e \leq p_0, \\ \frac{2(N_e-1)}{UN} + S \left( N_e - 1, \frac{\pi}{N} \right) - \frac{1}{UN} S \left( N_e - 1, \frac{2\pi}{N} \right) & \text{for } N_e > p_0, \end{cases}$$

(6.2)

where $p_0$ is the integer part of the expression

$$\frac{N}{\pi} \text{arccos} \left( \frac{UN}{4} - \sqrt{\left( \frac{UN}{4} \right)^2 - \frac{N - 2}{2}} \right)$$

(6.3)

and can be calculated from the condition $\varepsilon_n < -\frac{2}{U}$ for each $n < p_0$. Comparing (6.2) 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 exist

$$U_c(N_e) = \frac{1}{S \left( N_e, \frac{\pi}{N+1} \right) - S \left( N_e - 1, \frac{\pi}{N} \right)} \left\{ \frac{1}{N+1} \left[ S(N_e, \frac{2\pi}{N+1} + 2N_e) - \frac{1}{N} \left[ S \left( N_e - 1, \frac{2\pi}{N} \right) + 2(N + N_e - 1) \right] \right] \right\}. \quad (6.4)$$

The critical interaction strength $U_c$ as a function of the electron- and ion-density ratio $n_e/(1 - n_i)$ is plotted in Fig. 5. 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]. Of course, since our results were obtained in the strong interaction limit using the perturbation theory, it is necessary to bound the phase diagram from below with some physical reasonable value of the interaction strength $U_0$, above which the perturbation procedure gives reasonable results. Tests which we made (see Fig. 2) show that this value should be relatively small ($U_0 \approx 5$).

The critical value $U_c$ (6.4) was obtained for the case when two connected clusters of unoccupied sites in the configuration $w_D$ were separated by two or more ions. Repeating the previous analysis for the case when these clusters are separated only by a single ion, one can directly show that this configuration has up to the order
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Fig. 5. The critical interaction strength $U_c$ as a function of the electron- and ion-density ratio $n_e/(1 - n_i)$.

$1/U$ the same energy spectrum as $\omega_D$, which again leads to (6.4). Finally, let us note that our estimate of the lower bound $U_c \equiv U^-$, below which the segregated phase cannot be the ground state of the one-dimensional Falicov-Kimball model, is better than the estimate of Brandt, who investigated stability of the segregated phase with respect to "evaporation" [8]. But 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 result for $U^-$ yields sharp bounds for the segregated state.

References