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Ground States of the Spinless Falicov–Kimball Model. II

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In this paper we continue our investigation of the ground states of the spinless Falicov–Kimball model in the plane of chemical potentials of the two sorts of particles involved. We obtain a number of general properties of the phase diagram. We also derive an expansion for large values of the coupling constant, from which we deduce results concerning particular states.

KEY WORDS: Falicov–Kimball model; ground-state phase diagram; large-U expansion.

1. INTRODUCTION

This paper is a complement to our earlier work,[1] in which we studied the zero-temperature phase diagram of the spinless Falicov–Kimball model. This model was originally proposed by Falicov and Kimball[2] to describe a metal–insulator transition in solids. Later it was realized that the Falicov–Kimball model is also of interest to study mixed-valence phenomena and crystallization effects.[3,4]

The system consists of noninteracting spinless fermions (here called electrons) on a lattice. These particles move in a potential assuming only two values $\pm U$ at each site (here interpreted as the presence or absence of a classical ion). The density of ions and electrons can vary and is controlled by the corresponding chemical potentials μ_i and μ_e.

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In ref. 1 we used the moment method of Tchebycheff and Markov to determine domains in the plane of chemical potentials where the configurations of ions which minimize the energy of the system can be found. However, this method yields domains whose boundaries extend to infinity, while it is intuitively clear that they should remain bounded. Here, in particular, we fill this gap.

In Section 2 we define the model. Then in consecutive subsections of Section 3 we present new results concerning the phase diagram together with their proofs. We also give a summary of the results previously obtained. Section 3.1 is devoted to symmetry and other general properties (independent of the value of the potential, of particular configurations of ions, and of the boundary conditions). Then in Section 3.2 we consider specific configurations of the ions, mainly the three following cases: the empty configuration, the fully occupied configuration, and the chessboard configuration. We consider the results obtained for the first two configurations particularly interesting. They reveal the distinguished role played by these two configurations in constructing an overall picture of the phase diagram. In particular, they imply that any other periodic configuration of ions can be a ground state only for chemical potentials which are strictly inside the domains represented in Figs. 1 and 2 (except for the trivial situation where all configurations have the same energy). For example, the chessboard configuration cannot be a ground state for values of μ_e which are inside the energy bands of the chessboard Hamiltonian. Finally, in Section 3.3 we derive an expansion of the ground-state energy with respect to U^{-1}. This expansion enables us to deduce some more details of the phase diagram for very large values of the potential. In particular, the results obtained in Section 3.3 prompt us to conjecture that the phase diagram of the 2-dimensional Falicov–Kimball model has a devil's-staircase structure.

2. THE SPINLESS FALICOV–KIMBALL MODEL

The model is defined on a finite cubic lattice $\Lambda \subset \mathbb{Z}^\nu$ by the Hamiltonian

$$H = \sum_{x,\, y \in \Lambda} t_{xy} a_x^+ a_y + 2U \sum_{x \in \Lambda} W(x)\, a_x^+ a_x - \mu_e N_e - \mu_i N_i \tag{1}$$

where a_x^+, a_x are the creation and annihilation operators for electrons at site x ($a_x^+ a_y + a_y a_x^+ = \delta_{xy}$). The hopping matrix element t_{xy} is given by $t_{xy} = 1$ if $|x-y| = 1$ and zero otherwise. The variable $W(x)$ is 1 or 0 according to whether the site x is occupied or unoccupied by an ion. N_e and N_i denote the numbers of electrons and ions, i.e.,

$$N_e = \sum_{x \in \Lambda} a_x^+ a_x, \qquad N_i = \sum_{x \in \Lambda} W(x) \tag{2}$$

and μ_e, μ_i are the corresponding chemical potentials.

For symmetry reasons it is convenient to introduce the spin variable $s_x = 2W(x) - 1$ ($s_x = \pm 1$) and to rewrite the Hamiltonian in the form

$$H(s) = \sum_{x,\, y \in \Lambda} h_{xy}(s)\, a_x^+ a_y - \tilde{\mu}_e N_e - (\tilde{\mu}_i + U)\, N_i(s) \tag{3}$$

where

$$h_{xy}(s) = t_{xy} + U s_x \delta_{xy} \tag{4}$$

is the matrix element of the single-particle operator

$$h(s) = T + US \tag{5}$$

and

$$\tilde{\mu}_e = \mu_e - U, \qquad \tilde{\mu}_i = \mu_i - U \tag{6}$$

In the following we shall concentrate on the ion subsystem. It is thus useful to introduce the effective interaction $F(s)$ between ions in the configuration s. This interaction is defined by means of the grand canonical partition function Z_Λ:

$$Z_\Lambda = \sum_{\{s\}} \operatorname{Tr} \exp[-\beta H(s)] = \sum_{\{s\}} \exp[-\beta F_\Lambda(s)] \tag{7}$$

The sum is over all possible ion configurations; the trace is over the $2^{|\Lambda|}$-dimensional electron Hilbert space.

The effective interaction $F_\Lambda(s)$ depends on the temperature β^{-1} and on the two chemical potentials $\tilde{\mu}_e$ and $\tilde{\mu}_i$. Since we want to consider only zero-temperature properties of the system, we introduce the zero-temperature energy in the configuration s:

$$\begin{aligned} E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s) &= \frac{1}{|\Lambda|} \lim_{\beta \to \infty} F_\Lambda(s) \\ &= \frac{1}{|\Lambda|} \sum_{\varepsilon(j,s) < \tilde{\mu}_e} [\varepsilon(j, s) - \tilde{\mu}_e] - (\tilde{\mu}_i + U)\, \rho_i(s) \end{aligned} \tag{8}$$

where $\varepsilon(j, s)$, $j = 1,..., |\Lambda|$, are the eigenvalues of $h(s)$ and $\rho_i(s) = (1/|\Lambda|)\, N_i(s)$ is the ion density in the configuration s.

The function $(\tilde{\mu}_e, \tilde{\mu}_i) \to E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s)$ is continuous and concave on the whole plane of chemical potentials and differentiable almost everywhere. Along the lines parallel to the $\tilde{\mu}_i$ axis this function is linear with the slope

$$\frac{\partial E_\Lambda}{\partial \tilde{\mu}_i}(\tilde{\mu}_e, \tilde{\mu}_i; s) = -\rho_i(s) \tag{9}$$

Along the lines parallel to the $\tilde{\mu}_e$ axis the function (8) is constant below the lower edge of the spectrum of $h(s)$ [$=\operatorname{spec} h(s)$] and strictly decreasing above this value. Its slope defines the electron density in the configuration s,

$$\frac{\partial E_\Lambda}{\partial \tilde{\mu}_e}(\tilde{\mu}_e, \tilde{\mu}_i; s) = -\rho_e^\Lambda(\tilde{\mu}_e; s) \tag{10}$$

everywhere except at the points of $\operatorname{spec} h(s)$.

In the next section we study the phase diagram in the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane. We consider mainly the ion subsystem, i.e., for a given point $(\tilde{\mu}_e, \tilde{\mu}_i)$, we look for the configurations s of ions which minimizes the energy density (8) (concerning the electron subsystem, we try only to control the density). This amounts to constructing the lower concave envelope of the set of functions $\{E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s)\}$, i.e.,

$$E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i) = \min_s \{E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s)\} \tag{11}$$

which is the *ground-state energy density* of our system at the point $(\tilde{\mu}_e, \tilde{\mu}_i)$. This function has the same properties as the functions $E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s)$, except that along the lines parallel to the $\tilde{\mu}_i$ axis it is piecewiese linear and along the lines parallel to the $\tilde{\mu}_e$ axis the lower edge of $\operatorname{spec} h(s)$ has to be replaced by $-2v - U$. Hence the *ground-state electron density* $\rho_e^\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$ and the *ground-state ion density* $\rho_i^\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$ are defined almost everywhere by the counterparts of (9), (10). To be more specific, we define the set of *finite-volume ground-state configurations* (g.s.c.) at $(\tilde{\mu}_e, \tilde{\mu}_i)$:

$$G_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i) = \{s' : E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s') = E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)\} \tag{12}$$

Obviously, at any point $(\tilde{\mu}_e, \tilde{\mu}_i)$ the set $G_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$ is nonempty. In general at $(\tilde{\mu}_e, \tilde{\mu}_i)$ the left and right partial derivatives of $E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$ are different:

$$\frac{\partial E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)}{\partial \tilde{\mu}_\alpha^-} = -\min_{s \in G_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)} \rho_\alpha^\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s) \tag{13}$$

$$\frac{\partial E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)}{\partial \tilde{\mu}_\alpha^+} = -\max_{s \in G_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)} \rho_\alpha^\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s), \qquad \alpha = i, e \tag{14}$$

The densities $\rho_\alpha^\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$ are defined if and only if the left and right derivatives are equal. This means, in particular, that $\rho_i^\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$ is defined if and only if $\rho_i(s)$ is the same for all $s \in G_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$.

In general one is interested in properties of the infinite system. Therefore, taking the thermodynamic limit $\Lambda \to \mathbb{Z}^\nu$, we define

$$E(\tilde{\mu}_e, \tilde{\mu}_i; s) = \lim_{\Lambda \to \mathbb{Z}^\nu} E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s) \tag{15}$$

and

$$E(\tilde{\mu}_e, \tilde{\mu}_i) = \lim_{\Lambda \to \mathbb{Z}^\nu} E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i) \tag{16}$$

Assuming the limits exist, these functions share the properties of their finite system counterparts (continuity, concavity, differentiability almost everywhere). At each point $(\tilde{\mu}_e, \tilde{\mu}_i)$ they have left and right derivatives that are limits as $\Lambda \to \mathbb{Z}^\nu$ of the corresponding finite system quantities. Finally, we define the set of g.s.c.:

$$G(\tilde{\mu}_e, \tilde{\mu}_i) = \{s: E(\tilde{\mu}_e, \tilde{\mu}_i) = \lim_{\Lambda \to \mathbb{Z}^\nu} E_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i; s)\} \tag{17}$$

The phase diagram is then a partition of the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane into domains with the same set $G(\tilde{\mu}_e, \tilde{\mu}_i)$ of ground-state configurations.

3. PROPERTIES OF THE PHASE DIAGRAM

The results obtained can be classified into three types:

1. Symmetry and general properties (valid for all values of the coupling constant and all configurations, and independent of the boundary conditions).
2. Results for specific configurations of the ions (s^+: $s_x = 1$ for all x; s^-: $s_x = -1$ for all x; and s_{cb}: $s_x s_y = -1$ for any pair of nearest neighbors; for $\nu = 2$, s_{cb} is a chessboardlike configuration).
3. Results obtained from the expansion of the effective interaction with respect to U^{-1}.

3.1. Symmetries of the Phase Diagram and General Properties

Property 1. If $s \in G(\tilde{\mu}_e, \tilde{\mu}_i)$ with densities ρ_e and ρ_i, then $-s \in G(-\tilde{\mu}_e, -\tilde{\mu}_i)$ with densities $1-\rho_e$ and $1-\rho_i$, respectively.

This is a consequence of the equalities

$$E(\tilde{\mu}_e, \tilde{\mu}_i; s) = E(-\tilde{\mu}_e, -\tilde{\mu}_i; -s) - (\tilde{\mu}_e + \tilde{\mu}_i)$$
$$\rho_e(\tilde{\mu}_e; s) = 1 - \rho_e(-\tilde{\mu}_e; -s) \tag{18}$$

which are obtained by means of the hole–particle transformation for both sorts of particles.[4] Therefore, it is sufficient to study the phase diagram in a half-plane of the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane, for instance, $\tilde{\mu}_e \geqslant 0$. For $\tilde{\mu}_e = \tilde{\mu}_i = 0$ the system is invariant under the hole–particle transformation and at this point $\rho_e = \rho_i = 1/2$.

Property 2. If $s \in G(\tilde{\mu}_e, \tilde{\mu}_i; U)$ with densities ρ_e and ρ_i, then $-s \in G(\tilde{\mu}_e, -\tilde{\mu}_i; -U)$ with densities ρ_e and $1 - \rho_i$, respectively.

This property is derived in a similar way as the previous one. It enables us to restrict our considerations to positive U. From now on, we assume $U > 0$.

It follows from the concavity of the function $(\tilde{\mu}_e, \tilde{\mu}_i) \to E(\tilde{\mu}_e, \tilde{\mu}_i)$ that the functions $\tilde{\mu}_e \to \rho_e(\tilde{\mu}_e, \tilde{\mu}_i)$ and $\tilde{\mu}_i \to \rho_i(\tilde{\mu}_e, \tilde{\mu}_i)$ are nondecreasing. However, slightly stronger statements can be formulated.

We consider first variations of ρ_i along vertical lines in the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane, i.e., constant $\tilde{\mu}_e$.

Property 3. For $\tilde{\mu}_i'' > \tilde{\mu}_i'$ and $s'' \in G(\tilde{\mu}_i'')$, then either $s'' \in G(\tilde{\mu}_i')$ or

$$\rho_i(s'') > \sup_{s \in G(\tilde{\mu}_i')} \rho_i(s)$$

Since $\tilde{\mu}_e$ is held constant, (8) yields

$$E(\tilde{\mu}_i''; s) = E(\tilde{\mu}_i'; s) - (\tilde{\mu}_i'' - \tilde{\mu}_i')\, \rho_i(s) \tag{19}$$

Therefore

$$\begin{aligned} &E(\tilde{\mu}_i''; s'') - E(\tilde{\mu}_i''; s') \\ &\quad = E(\tilde{\mu}_i'; s'') - E(\tilde{\mu}_i'; s') - (\tilde{\mu}_i'' - \tilde{\mu}_i')[\rho_i(s'') - \rho_i(s')] \end{aligned} \tag{20}$$

For $s'' \in G(\tilde{\mu}_i'')$ the left-hand side of (20) is nonpositive for all s'. If $s'' \notin G(\tilde{\mu}_i')$, then $E(\tilde{\mu}_i'; s'') - E(\tilde{\mu}_i'; s') \geqslant \delta > 0$ for any s' in $G(\tilde{\mu}_i')$ and thus $\tilde{\mu}_i'' > \tilde{\mu}_i'$ implies $\rho_i(s'') > \rho_i(s')$ for any s' in $G(\tilde{\mu}_i')$.

Then, using Properties 9 and 11 derived below, for any $\tilde{\mu}_e$ in the strip

$$|\tilde{\mu}_e| \leqslant \bar{\mu}_e = \max\{\sigma, U - 2v\}$$

(where σ is given in Appendix B), there exist values of $\tilde{\mu}_i$ where the chessboard configurations are the only periodic g.s.c.; we thus have the following consequence of Property 3.

Corollary 1. If $|\tilde{\mu}_e| \leqslant \tilde{\mu}_e$, then either $\rho_i = 1/2$ and the chessboard configuration is the only periodic g.s.c., or $\rho_i \neq 1/2$. Furthermore, for the chessboard configuration, $\rho_e = 1/2$, since $\tilde{\mu}_e$ is in the gap of spec $h(s_{cb})$.

A property similar to Property 3 holds along horizontal lines in the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane, i.e., constant $\tilde{\mu}_i$:

Property 4. For $\tilde{\mu}''_e > \tilde{\mu}'_e$ and $s'' \in G(\tilde{\mu}''_e)$, then either $s'' \in G(\tilde{\mu}'_e)$ or

$$\rho_e(\tilde{\mu}''_e; s'') > \sup_{s \in G(\tilde{\mu}'_e)} \rho_e(\tilde{\mu}'_e; s)$$

Indeed, if the function $E(\tilde{\mu}_e)$ is nonlinear in the interval $[\tilde{\mu}'_e, \tilde{\mu}''_e]$, the result is immediate, since concavity, (13), and $\tilde{\mu}''_e > \tilde{\mu}'_e$ imply

$$\sup_{s \in G(\tilde{\mu}'_e)} \rho_e(\tilde{\mu}'_e; s) < \inf_{s \in G(\tilde{\mu}''_e)} \rho_e(\tilde{\mu}''_e; s) \leqslant \rho_e(\tilde{\mu}''_e; s)$$

On the other hand, if $E(\tilde{\mu}_e)$ is linear on this interval, and $s'' \notin G(\tilde{\mu}'_e)$, then the result follows again from concavity.

Before we formulate the next property, we need to make a few observations. Let s be some ion configuration and let us add to s a certain number of ions to obtain $\bar{s}$. This implies that $h(\bar{s}) = h(s) + U\,\Delta S$, where ΔS is a positive operator. Consequently, $\varepsilon(j, \bar{s}) \geqslant \varepsilon(j, s)$, $j = 1,..., |\Lambda|$, and the number of eigenvalues of $h(\bar{s})$ below a certain level $\tilde{\mu}_e$ is not greater than the number of eigenvalues of $h(s)$ below this level. Introducing the support of s $(= \{x \in \Lambda \mid s_x = 1\} = \operatorname{supp} s)$, we then have

$$\rho_e(\tilde{\mu}_e; \bar{s}) \leqslant \rho_e(\tilde{\mu}_e; s) \qquad \text{if} \quad \operatorname{supp} \bar{s} \supset \operatorname{supp} s \tag{21}$$

In particular, for any s,

$$\rho_e(\tilde{\mu}_e; s^+) \leqslant \rho_e(\tilde{\mu}_e; s) \leqslant \rho_e(\tilde{\mu}_e; s^-) \tag{22}$$

The next observation is that we can express $E(\tilde{\mu}_e, \tilde{\mu}_i; s)$ in terms of $\rho_e(\tilde{\mu}_e; s)$:

$$E(\tilde{\mu}_e, \tilde{\mu}_i; s) = -\int_{-\infty}^{\tilde{\mu}_e} d\mu\, \rho_e(\mu; s) - (\tilde{\mu}_i + U)\,\rho_i(s) \tag{23}$$

Therefore, for any s, $\bar{s}$, the inequality $E(\tilde{\mu}_e, \tilde{\mu}_i; \bar{s}) < E(\tilde{\mu}_e, \tilde{\mu}_i; s)$ is satisfied if and only if

$$\int_{-\infty}^{\tilde{\mu}_e} d\mu\, [\rho_e(\mu; s) - \rho_e(\mu; \bar{s})] < (\tilde{\mu}_i + U)[\rho_i(\bar{s}) - \rho_i(s)] \tag{24}$$

Now, if s and $\bar{s}$ are such that $\operatorname{supp} s \subset \operatorname{supp} \bar{s}$, then $\rho_e(\tilde{\mu}_e; s) - \rho(\tilde{\mu}_e; \bar{s}) \geqslant 0$, $\rho_i(\bar{s}) > \rho_i(s)$, and (24) yield

$$\text{if} \quad E(\tilde{\mu}_e''; \bar{s}) < E(\tilde{\mu}_e''; s), \quad \text{then for} \quad \tilde{\mu}_e' < \tilde{\mu}_e'' \quad \text{we have}$$

$$\int_{-\infty}^{\tilde{\mu}_e'} d\mu \, [\rho_e(\mu; s) - \rho_e(\mu; \bar{s})] \leqslant \int_{-\infty}^{\tilde{\mu}_e''} d\mu \, [\rho_e(\mu; s) - \rho_e(\mu; \bar{s})]$$
$$< (\tilde{\mu}_i + U)[\rho_i(\bar{s}) - \rho_i(s)] \tag{25}$$

i.e., $E(\tilde{\mu}_e'; \bar{s}) < E(\tilde{\mu}_e'; s)$. Summing up, we have the following result.

Lemma 1. If $\operatorname{supp} \bar{s} \supset \operatorname{supp} s$ and $E(\tilde{\mu}_e'; \bar{s}) > E(\tilde{\mu}_e'; s)$, then $E(\tilde{\mu}_e''; \bar{s}) > E(\tilde{\mu}_e''; s)$ for $\tilde{\mu}_e'' > \tilde{\mu}_e'$.

We are now ready to establish the following result.

Property 5. For $\tilde{\mu}_e'' > \tilde{\mu}_e'$ and $s'' \in G(\tilde{\mu}_e'')$, then either $s'' \in G(\tilde{\mu}_e')$ or s'' cannot be obtained from $s' \in G(\tilde{\mu}_e')$ by adding ions.

Suppose, on the contrary, that $\operatorname{supp} s'' \supset \operatorname{supp} s'$ for some $s' \in G(\tilde{\mu}_e')$. If $s'' \notin G(\tilde{\mu}_e')$, then $E(\tilde{\mu}_e'; s'') > E(\tilde{\mu}_e'; s')$; hence, according to Lemma 1, we have also $E(\tilde{\mu}_e''; s'') > E(\tilde{\mu}_e''; s')$, which is in contradiction with the fact that $s'' \in G(\tilde{\mu}_e'')$.

This last property together with Property 3 implies immediately the following result.

Corollary 2. If $s^+ \in G(\tilde{\mu}_e, \tilde{\mu}_i)$, then $s^+ \in G(\tilde{\mu}_e', \tilde{\mu}_i')$ for every $(\tilde{\mu}_e', \tilde{\mu}_i')$ contained in the closed quadrant intersection of the two half-planes $\tilde{\mu}_e' \leqslant \tilde{\mu}_e$ and $\tilde{\mu}_i' \geqslant \tilde{\mu}_i$.

A similar property holds for s^- with $\tilde{\mu}_e' \geqslant \tilde{\mu}_e$ and $\tilde{\mu}_i' \leqslant \tilde{\mu}_i$.

3.2. Results for Specific Configurations

Let us start with a few remarks concerning the spectrum of $h(s)$. For $U=0$, $h(s)=T$, and its spectrum is in $[-2v, 2v]$. For $U \neq 0$ and any s, $\operatorname{spec} h(s) \subset [-2v-U, 2v+U]$. The two translationally invariant configurations s^+ and s^- have particularly simple spectra which are obtained by translation by $\pm U$ of spec T. As might be expected, these configuration fill most of the $(\tilde{\mu}_e, \tilde{\mu}_i)$ phase diagram.

We quote first properties claiming that s^+ and s^- fill a few half-planes of the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane. The intersection of the complements of these planes is a bounded rectangular domain around the origin which is the only domain where other configurations of ions can be g.s.c. First we consider two vertical half-planes.

Property 6. Let $\tilde{\mu}_e > U + 2v$. For $\tilde{\mu}_i > U$, s^+ is the unique periodic g.s.c.; for $\tilde{\mu}_i < U$, s^- is the unique periodic g.s.c.; for $\tilde{\mu}_i = U$, any s is a g.s.c.

To establish this property, it is sufficient to notice that if $\tilde{\mu}_e \geqslant U + 2v$, then $E(\tilde{\mu}_e, \tilde{\mu}_i; s) = -(\tilde{\mu}_i - U)\,\rho_i(s) - (U + \tilde{\mu}_e)$, since $(1/|\Lambda|)\operatorname{Tr} S = 2\rho_i(s) - 1$, and $\operatorname{Tr} T = 0$.

Using Property 1, we can extend this property for negative values of $\tilde{\mu}_e$: Let $\tilde{\mu}_e < -U - 2v$. For $\tilde{\mu}_i > -U$, s^+ is the unique periodic g.s.c.; for $\tilde{\mu}_i < -U$, s^- is the unique periodic g.s.c.; for $\tilde{\mu}_i = -U$, any s is a g.s.c.

Now we consider two horizontal half-planes.

Property 7. For $\tilde{\mu}_i > U$, s^+ is the unique periodic g.s.c.; for $\tilde{\mu}_i < -U$, s^- is the unique periodic g.s.c. For $\tilde{\mu}_i = U$ (resp. $-U$), s^+ (resp. s^-) is a g.s.c.

Indeed, according to (22) and (23),

$$\begin{aligned} &E(\tilde{\mu}_e, \tilde{\mu}_i; s) - E(\tilde{\mu}_e, \tilde{\mu}_i; s^-) \\ &\quad = -(\tilde{\mu}_i + U)\,\rho_i(s) + \int_{-\infty}^{\tilde{\mu}_e} d\mu'\,[\rho_e(\mu', \tilde{\mu}_i; \bar{s}) - \rho_e(\mu', \tilde{\mu}_i; s)] \\ &\quad \geqslant -(\tilde{\mu}_i + U)\,\rho_i(s) \geqslant 0 \end{aligned} \tag{26}$$

for any s and $\tilde{\mu}_i \leqslant -U$. The above inequality becomes strict for $\tilde{\mu}_i < -U$ and $\rho_i(s) \neq 0$. Applying Property 1, we get a similar result for s^+.

The set of points $(\tilde{\mu}_e, \tilde{\mu}_i)$ where the g.s.c. are not known has been reduced to the rectangle $D = [-U - 2v, U + 2v] \times [-U, U]$. We will show that this set is considerably smaller, since s^+ and s^- continue to be the g.s.c. inside D.

It was proved in refs. 4 and 5 that at the origin s_{cb} are the unique periodic g.s.c. More information was obtained in ref. 1. By means of the moment method of Tchebycheff and Markov we obtain the following regions in D, where the configurations s^+, s^-, and s_{sb} are the g.s.c. (Fig. 1).

Property 8. For $\tilde{\mu}_e$ in the vertical stripe $-U - 2v \leqslant \tilde{\mu}_e \leqslant U - 2v$ and $\tilde{\mu}_i > f_+(\tilde{\mu}_e)$, s^+ is the unique periodic g.s.c.; for $\tilde{\mu}_i = f_+(\tilde{\mu}_e)$, it is a g.s.c.

The precise form of the function f_+ is given in Appendix B.

Actually, in ref. 1 we considered the case $v = 2$. However, the results remain valid for $v \geqslant 2$. The necessary generalization of the expressions used in ref. 1 are given in Appendix A.

The counterpart of Property 8 for s^- follows from Property 1.

Property 9. For $-\sigma \leqslant \tilde{\mu}_e \leqslant 0$ and

$$\tilde{\mu}_e[C(U) - D(U)] + b(U) \leqslant \tilde{\mu}_i \leqslant \tilde{\mu}_e[C(U) + D(U)] + b(U)$$

s_{cb} are the unique periodic g.s.c.

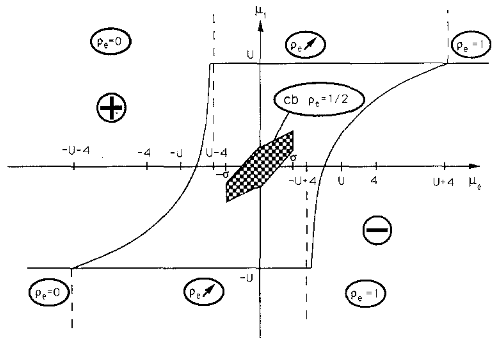


Fig. 1. Location of the s^+, s^-, and s_{cb} configurations in the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane for $v = 2$.

The coefficients $C(U)$, $D(U)$, $b(U)$ and the parameter σ are given in Appendix B.

Again Property 1 is used to extend the above domain to positive values of $\tilde{\mu}_e$. Since $\sigma < U/3$, then $-\sigma$ is in the gap of the spectrum of $h(s_{cb})$ and $\rho_e = 1/2$.

The above properties of the configurations s^+, s^-, and s_{cb} are summarized in Fig. 1.

The properties listed above are valid for all U. However if U is sufficiently large, new general (configuration-independent) features of spec $h(s)$ arise. They enable us to formulate additional properties of the phase diagram.

Using the operator inequality[4]

$$h^2(s) \geqslant (U - 2v)^2 \qquad \text{if} \quad U \geqslant 2v \tag{27}$$

we conclude that the eigenvalues $\varepsilon(j, s)$, $j = 1,..., |\Lambda|$, of $h(s)$ satisfy the inequality

$$|\varepsilon(j, s)| \geqslant |U - 2v| \qquad \text{if} \quad U \geqslant 2v \tag{28}$$

This means that for $U > 2v$, a gap $[-U + 2v, U - 2v]$ opens in the spectrum of $h(s)$ for any s.

Property 10 $(U > 2v)$. If $\tilde{\mu}_e$ is in the gap, i.e., $|\tilde{\mu}_e| < U - 2v$, then for any $s \in G(\tilde{\mu}_e, \tilde{\mu}_i; U)$, we have

$$\rho_e(s) + \rho_i(s) = 1$$

This property is an immediate consequence of the following lemma.

Lemma 2. Let $U > 2v$ and $N_i(s)$ denote the number of ions in s; then the number of negative eigenvalues of $h(s)$ is $n_-(s) = |\Lambda| - N_i(s)$. The number of positive eigenvalues of $h(s)$ is $n_+(s) = N_i(s)$.

To establish this lemma, we adapt an argument from the proof of Theorem 2.1 in ref. 4. We note that for any configuration s we have the orthogonal decomposition of the single-electron Hilbert space:

$$\mathscr{H}(\Lambda) = \mathscr{H}(\operatorname{supp} s) \oplus \mathscr{H}(\Lambda \backslash \operatorname{supp} s)$$

where $\mathscr{H}(\operatorname{supp} s)$ is generated by vectors whose support is in $\operatorname{supp} s$, $\dim \mathscr{H}(\operatorname{supp} s) = N_i(s)$. If $U > 2v$, then zero is not an eigenvalue of $h(s)$ for any s (28); therefore,

$$n_-(s) + n_+(s) = |\Lambda| \tag{29}$$

This induces another orthogonal decomposition:

$$\mathscr{H}(\Lambda) = \mathscr{H}_+(s) \oplus \mathscr{H}_-(s)$$

where $\mathscr{H}_+(s)$ $[\mathscr{H}_-(s)]$ is the subspace generated by the eigenvectors of $h(s)$ whose eigenvalues are positive (negative), $\dim \mathscr{H}_+(s) = n_+(s)$. Suppose that $n_-(s) < |\Lambda| - N_i(s)$. Then there is $\varphi \in \mathscr{H}(\Lambda \backslash \operatorname{supp} s) \cap \mathscr{H}_+(s)$. For this φ we have

$$(\varphi, h(s)\varphi) > 0$$

and

$$\begin{aligned}(\varphi, h(s)\varphi) &= (\varphi, T\varphi) + U(\varphi, S\varphi)\\ &\leqslant \|T\| \, \|\varphi\|^2 - U \, \|\varphi\|^2 = (2v - U) \, \|\varphi\|^2 < 0\end{aligned} \tag{30}$$

which is a contradiction. Thus, $n_-(s) \geqslant |\Lambda| - N_i(s)$. A similar reasoning gives $n_+(s) \geqslant |\Lambda| - N_i(s)$. These two inequalities together with (29) conclude the proof.

Property 11 ($U > 2v$). Let $\tilde{\mu}_e$, $\tilde{\mu}'_e$ be in the gap, i.e., $|\tilde{\mu}_e|$, $|\tilde{\mu}'_e| < U - 2v$; then $G(\tilde{\mu}'_e, \tilde{\mu}'_i) = G(\tilde{\mu}_e, \tilde{\mu}_i)$ if $\tilde{\mu}'_e - \tilde{\mu}'_i = \tilde{\mu}_e - \tilde{\mu}_i$, i.e., the g.s.c. are the same on the lines $\tilde{\mu}_e - \tilde{\mu}_i = \text{const}$.

Indeed, if $\tilde{\mu}_e$ is in the gap, then the sum in (8) can be taken over $\varepsilon(j, s) < 0$. Since

$$\frac{1}{|\Lambda|} \sum_{\varepsilon(j,s) < 0} \varepsilon(j, s) = U\rho_i(s) - \frac{1}{2\,|\Lambda|} \operatorname{Tr} |h(s)| - \frac{U}{2}$$

and $\rho_e(\tilde{\mu}_e; s) = 1 - \rho_i(s)$ (Property 10), the energy (8) becomes

$$E_A(\tilde{\mu}_e, \tilde{\mu}_i; s) = (\tilde{\mu}_e - \tilde{\mu}_i)\, \rho_i(s) - \frac{1}{2\,|A|} \operatorname{Tr} |h(s)| - \left(\tilde{\mu}_e + \frac{U}{2}\right) \qquad (31)$$

Therefore the difference $E_A(\tilde{\mu}_e, \tilde{\mu}_i; s') - E_A(\tilde{\mu}_e, \tilde{\mu}_i; s)$ is constant along the lines $\tilde{\mu}_e - \tilde{\mu}_i = \text{const.}$

If $U > 2v$, Property 11 together with Property 9 enables us to extend the domain where s_{cb} are the g.s.c. Namely, s_{cb} are the g.s.c. in the parallelogram obtained by translating the segment that is the intersection of the $\tilde{\mu}_e = 0$ line with the region described in Property 9 across the gap parallel to the $\tilde{\mu}_e = \tilde{\mu}_i$ line.

The consequences of Properties 10 and 11 are summarized in Fig. 2.

To conclude this section, we shall show that for any ion configuration s there exists a rectangle in the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane, strictly inside D, such that s cannot be a g.s.c. for values of $(\tilde{\mu}_e, \tilde{\mu}_i)$ outside this rectangle.

Property 12. 1. For any configuration s there exist critical values $\tilde{\mu}_e^c(s)$ in $]-U-2v, U+2v[$ and $\tilde{\mu}_i^c(s)$ in $]-U, U[$ such that (Fig. 3)

$$E(s^+) = E(s^-) = E(s) \qquad \text{for} \quad \tilde{\mu}_e = \tilde{\mu}_e^c(s), \quad \tilde{\mu}_i = \tilde{\mu}_i^c(s)$$

Furthermore, for any $s \neq s^{\pm}$, then $s \notin G(\tilde{\mu}_e, \tilde{\mu}_i)$ if $(\tilde{\mu}_e, \tilde{\mu}_i)$ is strictly inside D, but outside the closed rectangle defined by the points $(\tilde{\mu}_e^c(s), \tilde{\mu}_i^c(s))$ and $(-\tilde{\mu}_e^c(-s), -\tilde{\mu}_i^c(-s))$.

2. If $s = -s$, the above rectangle is centered at the origin.

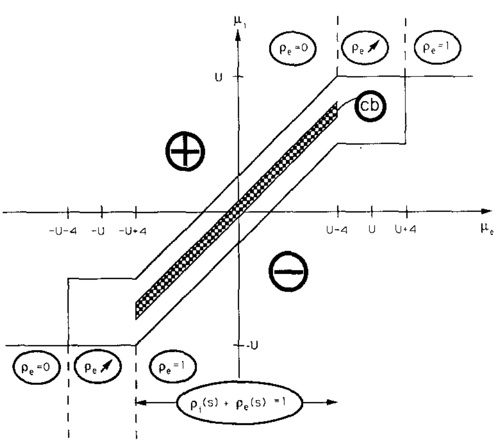


Fig. 2. Phase diagram for $U > 2v$, $v = 2$.

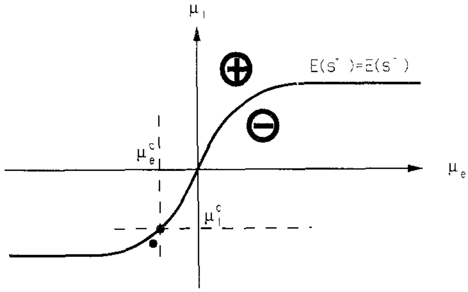


Fig. 3. The curve $f_+(\tilde{\mu}_e)$ defined by $E(s^+) = E(s^-)$.

Let us first recall that for $\tilde{\mu}_e \geqslant U + 2v$, we already know that $E(s^+) = E(s^-) = E(s)$ if $\tilde{\mu}_i = U$; for $\tilde{\mu}_e < -(U + 2v)$ the same is true if $\tilde{\mu}_i = -U$.

We shall establish this proposition by proving several simple lemmas.

From (23), together with the value of E for $\tilde{\mu}_e = U + 2v$, we obtain first

$$\int_{-\infty}^{U+2v} d\mu\, \rho_e(\mu; s) = 2v + 2U[1 - \rho_i(s)] \tag{32}$$

Then, from the symmetry properties

$$\begin{aligned} \rho_e(\tilde{\mu}_e; s) + \rho_e(-\tilde{\mu}_e, -s) &= 1 \\ \rho_i(s) + \rho_i(-s) &= 1 \end{aligned} \tag{33}$$

and (32) we have

$$\begin{aligned} &E(\tilde{\mu}_e, \tilde{\mu}_i; s) - E(\tilde{\mu}_e, \tilde{\mu}_i; -s) \\ &\quad = -\tilde{\mu}_e - \tilde{\mu}_i[1 - 2\rho_i(-s)] + \int_{-\tilde{\mu}_e}^{\tilde{\mu}_e} d\mu\, \rho_e(\mu; -s) \end{aligned} \tag{34}$$

Therefore $E(\tilde{\mu}_e, \tilde{\mu}_i; s) = E(\tilde{\mu}_e, \tilde{\mu}_i; -s)$ if and only if

$$\tilde{\mu}_i[1 - 2\rho_i(-s)] = -\tilde{\mu}_e + \int_{-\tilde{\mu}_e}^{\tilde{\mu}_e} d\mu\, \rho_e(\mu; -s) \tag{35}$$

Furthermore, the function $\tilde{\mu}_i = \tilde{\mu}_i(\tilde{\mu}_e; s)$ defined by (35) is nondecreasing with $\tilde{\mu}_e$ if and only if $\rho_e(\tilde{\mu}_e; -s) + \rho_e(-\tilde{\mu}_e, -s) \geqslant 1$, i.e., if $\rho_e(\tilde{\mu}_e; -s) \geqslant \rho_e(\tilde{\mu}_e; s)$. This will be in particular the case for $s = s^+$; indeed, $\rho_e(\tilde{\mu}_e; s^-) = \rho_e(\tilde{\mu}_e + 2U; s^+) \geqslant \rho_e(\tilde{\mu}_e; s^+)$, since ρ_e is nondecreasing with $\tilde{\mu}_e$. Therefore we have the following result.

Lemma 3. The equation $E(\tilde{\mu}_e, \tilde{\mu}_i; s) = E(\tilde{\mu}_e, \tilde{\mu}_i; -s)$ defines a function $\tilde{\mu}_i = f_s(\tilde{\mu}_e)$ which divides the $(\tilde{\mu}_e, \tilde{\mu}_i)$ plane into two domains, one where $E(s) < E(-s)$ the other where $E(-s) < E(s)$. Furthermore, $f_s(\tilde{\mu}_e) = -f_s(-\tilde{\mu}_e)$ and $f_s(\tilde{\mu}_e) = U$ for $\tilde{\mu}_e \geqslant \sup \operatorname{spec} h(s)$. The curve $\tilde{\mu}_i = f_+(\tilde{\mu}_e)$ associated with $E(s^+) = E(s^-)$ is strictly increasing for $\tilde{\mu}_e \in [-U-2v, U+2v]$.

Let us then introduce the following definitions: with s any periodic configuration we associate first the function

$$G_s(\tilde{\mu}_e) = -\int_{-\infty}^{\tilde{\mu}_e} d\mu\, \rho_e(\mu; s) \tag{36}$$

i.e.,

$$\begin{aligned} G_s(\tilde{\mu}_e) &= E(\tilde{\mu}_e, \tilde{\mu}_i; s) + (\tilde{\mu}_i + U)\, \rho_i(s) \\ &= \lim_{\Lambda \to \infty} \frac{1}{|\Lambda|} \sum_{\varepsilon_j(s) \leqslant \tilde{\mu}_e} [\varepsilon_j(s) - \tilde{\mu}_e] \end{aligned} \tag{37}$$

Notice that

$$\begin{aligned} &\text{for } \tilde{\mu}_e \geqslant \sup \operatorname{spec} h(s): \quad G_s(\tilde{\mu}_e) = U[2\rho_i(s) - 1] - \tilde{\mu}_e \\ &\text{for } \tilde{\mu}_e \leqslant \inf \operatorname{spec} h(s): \quad G_s(\tilde{\mu}_e) = 0 \end{aligned}$$

Since

$$\inf \operatorname{spec} h(s) > \inf \operatorname{spec} h(s^-) = -2v - U$$

we can define $\tilde{\mu}_e^c = \tilde{\mu}_e^c(s)$ and $\tilde{\mu}_i^c = \tilde{\mu}_i^c(s)$ by the equations

$$G_s(\tilde{\mu}_e^c) = [1 - \rho_i(s)]\, G_-(\tilde{\mu}_e^c) + \rho_i(s)\, G_+(\tilde{\mu}_e^c) \tag{38}$$

$$G_s(\tilde{\mu}_e) > [1 - \rho_i(s)]\, G_-(\tilde{\mu}_e) + \rho_i(s)\, G_+(\tilde{\mu}_e), \qquad -2v - U < \tilde{\mu}_e < \tilde{\mu}_e^c \tag{39}$$

and

$$(\tilde{\mu}_i^c + U) = G_+(\tilde{\mu}_e^c) - G_-(\tilde{\mu}_e^c) \tag{40}$$

Let us remark that for $\tilde{\mu}_e \geqslant U + 2v$

$$G_s(\tilde{\mu}_e) = U[2\rho_i(s) - 1] - \tilde{\mu}_e \qquad \text{for all } s$$

and thus

$$G_s(\tilde{\mu}_e) = [1 - \rho_i(s)]\, G_-(\tilde{\mu}_e) + \rho_i(s)\, G_+(\tilde{\mu}_e) \qquad \text{for} \quad |\tilde{\mu}_e| \geqslant U + 2v$$

On the other hand,

$$G_s(\tilde{\mu}_e) > [1-\rho_i(s)]\, G_-(\tilde{\mu}_e) + \rho_i(s)\, G_+(\tilde{\mu}_e)$$
$$\text{for}\quad \tilde{\mu}_e \in\,]2v-U, \inf\operatorname{spec} h(s)] \cup [\sup\operatorname{spec} h(s), 2v+U[$$

and thus

$$\begin{aligned} -2v-U < \tilde{\mu}_e^c &\leqslant 2v+U \\ -U < \tilde{\mu}_i^c &\leqslant U \end{aligned} \tag{41}$$

Lemma 4. For any periodic configuration s, we have

$$E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s^+) = E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s^-) = E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s)$$

Indeed, from (37),

$$\begin{aligned} E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s^+) &= G_+(\tilde{\mu}_e^c) - (\tilde{\mu}_i^c + U) \\ E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s^-) &= G_-(\tilde{\mu}_e^c) \end{aligned} \tag{42}$$

together with (40), this gives $E(s^+) = E(s^-)$.

Moreover,

$$E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s) = G_s(\tilde{\mu}_e^c) - (\tilde{\mu}_i^c + U)\, \rho_i(s)$$

and (38) yield

$$E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s) = [1-\rho_i(s)]\, E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s^-) + \rho_i(s)\, E(\tilde{\mu}_e^c, \tilde{\mu}_i^c; s^+)$$

which concludes the proof.

Lemma 5. For any periodic configuration s, then $s \notin G(\tilde{\mu}_e, \tilde{\mu}_i)$ for $\tilde{\mu}_e < \tilde{\mu}_e^c(s)$ and any $\tilde{\mu}_i$.

Indeed for $\tilde{\mu}_e < \tilde{\mu}_e^c(s)$, (39) yields

$$E(\tilde{\mu}_e, \tilde{\mu}_i; s) > [1-\rho_i(s)]\, E(\tilde{\mu}_e, \tilde{\mu}_i; s^-) + \rho_i(s)\, E(\tilde{\mu}_e, \tilde{\mu}_i; s^+) \tag{43}$$

Therefore

$$E(\tilde{\mu}_e, \tilde{\mu}_i; s) > \min\{E(s^+), E(s^-)\}$$

Lemma 6. For any periodic configuration s, then $s \notin G(\tilde{\mu}_e, \tilde{\mu}_i)$ for $\tilde{\mu}_i < \tilde{\mu}_i^c(s)$ and any $\tilde{\mu}_e$.

Indeed, let us consider $\tilde{\mu}_i' < \tilde{\mu}_i^c(s)$ and $\tilde{\mu}_e' \in [g_+(\tilde{\mu}_i'), \tilde{\mu}_e^c]$ (see Fig. 3), where $\tilde{\mu}_e = g_+(\tilde{\mu}_i)$ is the curve defined by $E(s^+) = E(s^-)$. For this value

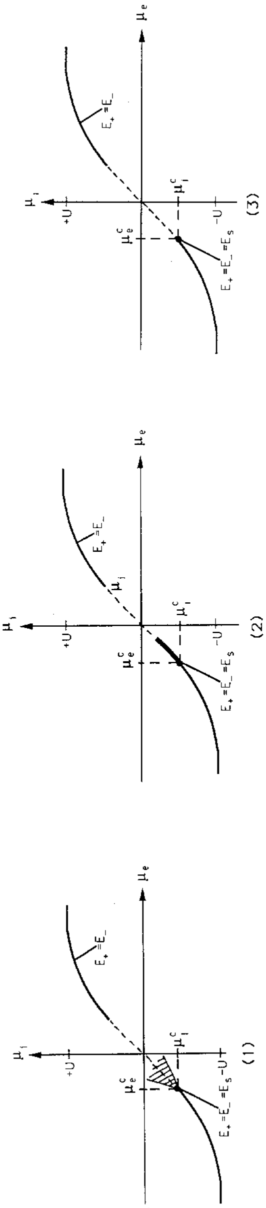


Fig. 4. Reduced phase diagram for s^+, s^-, and s around $(\tilde{\mu}_e^c, \tilde{\mu}_i^c)$.

$(\tilde{\mu}'_e, \tilde{\mu}'_i)$ we know that $E(\tilde{\mu}'_e, \tilde{\mu}'_i; s^-) < E(\tilde{\mu}'_e, \tilde{\mu}'_i; s)$ and thus Lemma 1 yields $E(\tilde{\mu}''_e, \tilde{\mu}'_i; s^-) < E(\tilde{\mu}''_e, \tilde{\mu}'_i; s)$ for any $\tilde{\mu}''_e > \tilde{\mu}'_e$.

Repeating the same argument with the configuration $-s$, and using the symmetry property, we conclude that

$$s \notin G(\tilde{\mu}_e, \tilde{\mu}_i) \qquad \text{for} \quad \tilde{\mu}_e > -\tilde{\mu}^c_e(-s) \quad (\text{any } \tilde{\mu}_i)$$
$$\text{and for} \quad \tilde{\mu}_i > -\tilde{\mu}^c_i(-s) \quad (\text{any } \tilde{\mu}_e)$$

All these results have been summarized in Property 12 above.

From the above lemmas we can also deduce the following result.

Corollary 3. (a) If $\tilde{\mu}^c_e(s) = U + 2v$, then s is a g.s.c. only on the trivial half-lines $|\tilde{\mu}_i| = U$, $|\tilde{\mu}_e| \geqslant U + 2v$.

(b) If $\tilde{\mu}^c_e(s) < U + 2v$, then either:

1. $G_s(\tilde{\mu}_e) < G_{\text{mix}}(\tilde{\mu}_e)$ for $\tilde{\mu}^c_e < \tilde{\mu}_e < \tilde{\mu}^c_e + \delta$; or
2. $G_s(\tilde{\mu}_e) = G_{\text{mix}}(\tilde{\mu}_e)$ for $\tilde{\mu}^c_e < \tilde{\mu}_e < \tilde{\mu}^c_e + \delta$; or
3. $G_s(\tilde{\mu}_e) > G_{\text{mix}}(\tilde{\mu}_e)$ for $\tilde{\mu}^c_e < \tilde{\mu}_e < \tilde{\mu}^c_e + \delta$;

where

$$G_{\text{mix}}(\tilde{\mu}_e) = [1 - \rho_i(s)]\, G_-(\tilde{\mu}_e) + \rho_i(s)\, G_+(\tilde{\mu}_e)$$

The corresponding reduced phase diagrams relating s^+, s^-, and s around $(\tilde{\mu}^c_e, \tilde{\mu}^c_i)$ are represented in Fig. 4, where (1) on the hatched domain, $E(s) < \min\{E(s^+), E(s^-)\}$; (2) on the thick like, $E(s^+) = E(s^-)$; (3) $(\tilde{\mu}^c_e, \tilde{\mu}^c_i)$ is the only point where $E(s) = E(s^+) = E(s^-)$.

Remark. For configurations such that $\rho_i(s) = 1/2$, Eq. (35) yields the following sum rule:

$$\tilde{\mu}_e = \int_{-\tilde{\mu}_e}^{\tilde{\mu}_e} d\mu\, \rho_e(\mu; s)$$

which should be useful as a test for numerical investigations.

For the special case of the chessboard configuration ($v = 2$), we can then give explicit values of $\tilde{\mu}_e$ for which s_{cb} cannot be a g.s.c.

Property 13. For the chessboard configuration in two dimensions, we have the lower bound $\tilde{\mu}^c_e(s_{cb}) > -U$ if $U > 4.12$, and thus s_{cb} cannot be a g.s.c. for $\tilde{\mu}_e$ smaller then $-U$, the lower edge of the gap of spec $h(s_{cb})$.

(We conjecture that this property remains valid for all values of $U > 4$.)

Indeed, if $U \geqslant 2$, then $G_+(\tilde{\mu}_e)=0$ for $\tilde{\mu}_e \leqslant -U$ and the slope of $\frac{1}{2}G_-(\tilde{\mu}_e=-U)$ is $-1/4$. The concavity property of $G_s(\tilde{\mu}_e)$ then yields a simple sufficient condition for $\tilde{\mu}_e^c(s_{cb})>-U$ (see Fig. 5), namely

$$G_{cb}(\tilde{\mu}_e=-U)>\frac{1}{2}G_-$$

$$2G_- - U < -(16+U^2)^{1/2} = \inf \operatorname{spec} h(s_{cb})$$

where $G_- = G_-(\tilde{\mu}_e=-U)$, from which we have

$$G_{cb}(\tilde{\mu}_e=-U)>\frac{1}{2}G_-$$

$$U>\frac{G_-^2-4}{G_-}$$

A straightforward calculation yields

$$G_- = -\frac{8}{\pi^2}$$

On the other hand, using a linear bound for the spectrum of s_{cb},

$$\varepsilon_j(cb)=[4(\cos k_x \pm \cos k_y)^2+U^2]^{1/2}<a+b\,|\cos k_x \pm \cos k_y|$$

we obtain

$$G_{cb}(\tilde{\mu}_e=-U)>-\frac{1}{2\pi}\left[U\left(1-\frac{8}{\pi}\right)+(16+U^2)^{1/2}+\left(\frac{8}{\pi}-2\right)(4+U^2)^{1/2}\right]$$

from which we have the bound $\tilde{\mu}_e^c(s_{cb})>-U$ if $U>4.12$.

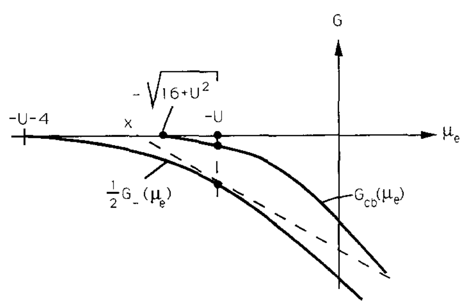


Fig. 5. Conditions for $\tilde{\mu}_e^c(s_{cb})>-U$ for $\nu=2$.

3.3. Expansion of the Effective Interaction in Powers of U^{-1} ($v=2$)

To gain some insight into the domain of the chemical potential plane where no rigorous results are available, we want to investigate in this last section the properties of the phase diagram in the limit of very large U. For this discussion we consider a finite two-dimensional square lattice and expand the effective interaction $E(\tilde{\mu}_e, \tilde{\mu}_i; s)$ in powers of U^{-1}. Then we shall search for the ground states of the approximate Hamiltonian to different orders. Although this approach does not yield rigorous results, it will give some insight into the expected structure of the phase diagram for large U.

To first order in U^{-1}, we have shown in ref. 1 that $E(\tilde{\mu}_e, \tilde{\mu}_i; s)$ is the Hamiltonian of the antiferromagnetic Ising model in a magnetic field, with $J = -1/4U$ and $h = \frac{1}{2}(\tilde{\mu}_e - \tilde{\mu}_i)$. It is well known that this model has two critical values of the magnetic field. Therefore, to first order in U^{-1}, we conclude that for $|\tilde{\mu}_e - \tilde{\mu}_i| < 2U^{-1}$ the chessboard configurations are the only ground states, while for $|\tilde{\mu}_e - \tilde{\mu}_i| > 2U^{-1}$ it is s^+ or s^-. Moreover, for $|\tilde{\mu}_e - \tilde{\mu}_i| = 2U^{-1}$ there is an infinite number of ground states with nonzero residual entropy. [Let us recall that in ref. 1 it was proved that for $|\tilde{\mu}_e - \tilde{\mu}_i| < U^{-1}$, s_{cb} are the unique g.s.c. and for $|\tilde{\mu}_e - \tilde{\mu}_i| > 4U^{-1}$, s^+ or s^- is the unique g.s.c., for the exact interaction $E(\tilde{\mu}_e, \tilde{\mu}_i; s)$.]

The question then arises: what is the effect of the higher-order terms? It is not difficult to see that all the even terms of the expansion vanish. Thus, to answer this question, it is necessary to go at least to order U^{-3}.

The first part of our derivation holds for any v. We assume that $U > 2v$ and $|\tilde{\mu}_e| < U - 2v$. In this case $E(\tilde{\mu}_e, \tilde{\mu}_i; s)$ is given by (31), and thus we have to expand $\operatorname{Tr} |h(s)|$:

$$\operatorname{Tr} |h(s)| = \operatorname{Tr}[h^2(s)]^{1/2} = \operatorname{Tr}[(T + US)^2]^{1/2} = U \operatorname{Tr}(1 + \Delta)^{1/2} \tag{44}$$

where

$$\Delta = U^{-1} J + U^{-2} T^2, \qquad J = TS + ST$$

To obtain the terms of order U^{-3}, we expand (44) to order 4 in powers of Δ:

$$\begin{aligned}\operatorname{Tr} |h(s)| &= U \operatorname{Tr}\left(1 + \frac{\Delta}{2} - \frac{\Delta^2}{8} + \frac{\Delta^3}{16} - \frac{5\Delta^4}{128}\right) + O(U^{-5}) \\ &= CU + \operatorname{Tr}\left(-\frac{1}{8}\frac{J^2}{U} + \frac{3}{16}\frac{J^2 T^2}{U^3} - \frac{5}{128}\frac{J^4}{U^3}\right) + O(U^{-5})\end{aligned}$$

$$= CU - \frac{1}{4U}\,\mathrm{Tr}(TS)^2 + \frac{1}{16U^3}\left[\mathrm{Tr}(T^3STS) + \frac{1}{2}\,\mathrm{Tr}(T^2S)^2 - \frac{5}{4}\,\mathrm{Tr}(TS)^4\right] + O(U^{-5}) \tag{45}$$

with C a constant independent of s. To compute the traces, we take $\nu = 2$. For this case we obtain

$$|\Lambda|\, E(\tilde{\mu}_e, \tilde{\mu}_i; s, U) = \frac{1}{2}(\tilde{\mu}_e - \tilde{\mu}_i) \sum_{x\in\Lambda} s_x + \left(\frac{1}{8U} - \frac{9}{32U^3}\right) \sum_{\substack{x, y\in\Lambda \\ |x-y|=1}} s_x s_y + \frac{3}{32U^3} \sum_{\substack{x, y\in\Lambda \\ |x-y|=\sqrt{2}}} s_x s_y + \frac{1}{16U^3} \sum_{\substack{x, y\in\Lambda \\ |x-y|=2}} s_x s_y + \frac{5}{16U^3} \sum_{P\in\Lambda} s_x s_y s_z s_w - \frac{U}{2} C - \frac{|\Lambda|}{2}(\tilde{\mu}_e + \tilde{\mu}_i + U) + O(U^{-5}) \tag{46}$$

The summation in the last term goes over the unit squares (=plaquettes) of Λ.

Since $\tilde{\mu}_e$ is inside the gap $[-U+4, U-4]$, we can take $\tilde{\mu}_e = 0$ without any loss of generality (see Property 11).

Introducing the variable δ defined by

$$\tilde{\mu}_i = \frac{2}{U} + \frac{\delta}{U^3}$$

and the rescaled Hamiltonian

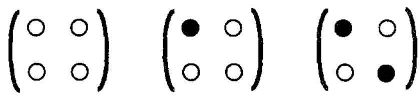
$$H'(s) = 16U^3\,|\Lambda|\, E(\tilde{\mu}_e = 0, \tilde{\mu}_i; s) + 8U^2\,|\Lambda|$$

we have

$$H'(s) = \sum_P \phi_P(s) + 2 \sum_{|x-y|=2} s_x s_y + O(U^{-2}) \tag{47}$$

where the four-body interaction is (see Fig. 6)

$$\phi_P(s) = \begin{cases} \varepsilon_1 = -8\delta - 7 & \text{if } s = \bar{s}_1 \\ \varepsilon_2 = -4\delta - 5 & \text{if } s = \bar{s}_2 \\ \varepsilon_3 = 29 & \text{if } s = \bar{s}_3 \\ O(U^2) & \text{otherwise} \end{cases}$$



($\bar{s}_1$) ($\bar{s}_2$) ($\bar{s}_3$)

Fig. 6. Configurations on plaquettes P; (●) -1, (○) $+1$.

Therefore, in the limit of large U we consider that the configurations with $\phi_P(s) = O(U^2)$ are forbidden, and we neglect the terms of order U^{-2} in (47). We then try to express $H'(s)$ as an m-potential,[8] i.e.,

$$H'(s) = \sum_{B \subset \Lambda} \phi_B(s)$$

where $s_0 \in G_\Lambda(\tilde{\mu}_e, \tilde{\mu}_i)$ if and only if $\phi_B(s_0) \leqslant \phi_B(s)$ for all B and s. For this purpose we rewrite $H'(s)$ in the form

$$H'(s) = \sum_P \tilde{\phi}_P(s) + \sum_B \phi_B(s)$$

where

$$\tilde{\phi}_P(s) = \phi_P(s) - \sum_{\substack{x,\, y \in P \\ |x-y|=1}} s_x s_y + \frac{h}{4} \sum_{x \in P} s_x$$

and $B = (x, y, z)$, where the three sites are nearest neighbors, vertical or horizontal,

$$\phi_B(s) = 2(s_x s_y + s_y s_z + s_x s_z) - \frac{h}{6} \sum_{x \in B} s_x$$

and h can be arbitrarily chosen. We then have for the 4-body potential (see Fig. 6)

$$\begin{aligned} \tilde{\varepsilon}_1 &= \tilde{\phi}_P(\bar{s}_1) = -8\delta - 15 + h \\ \tilde{\varepsilon}_2 &= \tilde{\phi}_P(\bar{s}_2) = -4\delta - 5 + h/2 \\ \tilde{\varepsilon}_3 &= \tilde{\phi}_P(\bar{s}_3) = 37 \end{aligned} \tag{48}$$

and for the 3-body potential (see Fig. 7)

$$\begin{aligned} e'_1 &= \phi_B(s'_1) = 6 - h/2 \\ e'_2 &= \phi_B(s'_2) = -2 - h/6 = \phi_B(s'_3) \\ e'_4 &= \phi_B(s'_4) = -2 + h/6 \end{aligned} \tag{49}$$

Fig. 7. Configurations on bonds $B = (x, y, z)$.

Therefore (see Fig. 8):

1. For $h = 84 + 8\delta < 0$, then $e'_4 < e'_2 < e'_1$, $\tilde{\varepsilon}_2 = \tilde{\varepsilon}_3 < \tilde{\varepsilon}_1$, and thus for $\delta < -21/2$, s_{cb} is the only g.s.c.
2. For $h = 84 + 8\delta \in]0, 24]$, then $e'_2 < e'_4$, $e'_2 \leqslant e'_1$, $\tilde{\varepsilon}_2 = \tilde{\varepsilon}_3 < \tilde{\varepsilon}_1$, and thus for $-21/2 < \delta \leqslant -15/2$, s_1 is the only g.s.c.
3. For $h = 84 + 8\delta = 0$, then $e'_2 = e'_4 < e'_1$, $\tilde{\varepsilon}_2 = \tilde{\varepsilon}_3 < \tilde{\varepsilon}_1$, and thus for $\delta = -21/2$, there is an infinite number of g.s.c., characterized by the condition that on each B the configuration s'_1 is forbidden.
4. For $h = 24$ and $2\delta > 1$, then $e'_1 = e'_2 < e'_4$, $\tilde{\varepsilon}_1 < \tilde{\varepsilon}_2$, and $\tilde{\varepsilon}_3$; thus, for $\delta > 1/2$, s^+ is the only g.s.c.
5. For $h = 24$ and $2\delta = 1$, $\tilde{\varepsilon}_1 = \tilde{\varepsilon}_2$, and thus for $\delta = 1/2$, there is an infinite number of g.s.c., characterized by the condition that on each plaquette there is at most one site with $s_x = -1$.

To find the g.s.c. in the remaining domain $\delta \in]-15/2, 1/2[$, we rewrite H' in the form

$$H' = \sum_P \phi''_P + \sum_{B'} \phi_{B'} + \sum_{B''} \phi_{B''} + \sum_{B'''} \phi_{B'''}$$

where B', B'', B''' denote bonds with 3, 6, and 8 points (see Fig. 9) and

$$\begin{aligned}
\phi_{B'} &= 2(s_x s_z + s_x s_y + s_y s_z) - 4 \sum_x s_x \\
\phi_{B''} &= K \sum_{|x-y|=2} s_x s_y + K \sum_{|x-y|=1} s_x s_y - 3K \sum_x s_x \\
\phi_{B'''} &= \frac{1}{2}(1-K) \sum_{|x-y|=2} s_x s_y - \frac{1}{2}(1-K) \sum_x s_x \\
\phi''_P &= \phi_P - 2 \sum_{\substack{|x-y|=1 \\ \text{hor.}}} s_x s_y - \frac{7}{2} K \sum_{|x-y|=1} s_x s_y + \left(4 + \frac{7}{2} K\right) \sum_x s_x
\end{aligned} \tag{50}$$

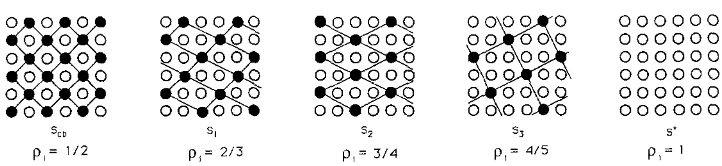


Fig. 8. Ground-state configurations at the order U^{-3} for $\nu = 2$.

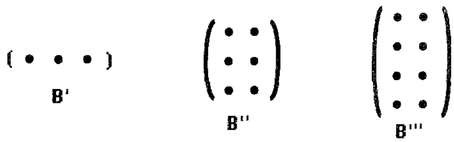


Fig. 9. Bonds B', B'', B'''.

and K can be arbitrarily chosen. We thus have (see Fig. 6)

$$\begin{aligned} \varepsilon_1'' &= \phi_P''(\bar{s}_1) = -8\delta + 5 \\ \varepsilon_2'' &= \phi_P''(\bar{s}_2) = -4\delta + 3 + 7K \\ \varepsilon_3'' &= \phi_P''(\bar{s}_3) = 33 + 14K \end{aligned} \tag{51}$$

For $7K = 2 - 4\delta$, we have $\varepsilon_1'' = \varepsilon_2'' < \varepsilon_3''$. On the other hand, for $0 < K < 1$, the configurations which minimize $\phi_{B'}$, $\phi_{B''}$, $\phi_{B'''}$ are those represented in Fig. 10. Therefore for $-5/4 < \delta < 1/2$, the configuration s_3 (Fig. 8) is the only g.s.c. These results are summarized in Fig. 11a. At the points $\mu_i = 2U^{-1} - (21/2)\,U^{-3}$ and $\mu_i = 2U^{-1} + \frac{1}{2}U^{-3}$ the number of ground states is infinite.

We were not able to find the g.s.c. for $\delta \in [-15/2, 5/4]$. However, looking at the average free energy for several different periodic configurations, we are led to conjecture that the ground states are those represented in Fig. 11b.

We thus obtained the following results:

1. At the order zero, the line $\tilde{\mu}_e = \tilde{\mu}_i$ separates the domain where s^- is the unique g.s.c. from the domain where s^+ is the unique g.s.c. On this line the number of g.s.c. is infinite.
2. At the order 1, this degeneracy is partially lifted and the line $\tilde{\mu}_e = \tilde{\mu}_i$ decomposes into two lines, $\tilde{\mu}_e = \tilde{\mu}_i \pm 2U^{-1}$, which separate the domains where s^-, s_{cb}, s_+ are the g.s.c. On both lines the number of g.s.c. is infinite.

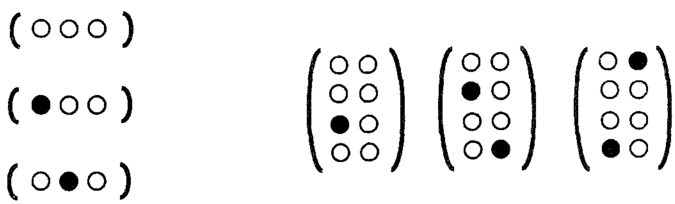


Fig. 10. Configurations on B', B'', B''' which minimize the potentials.

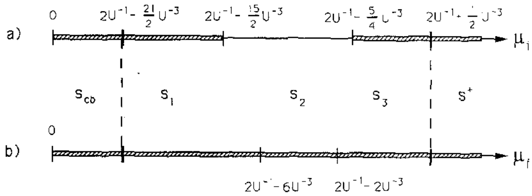


Fig. 11. (a) Phase diagram obtained at the order U^{-3}; (b) phase diagram conjectured at the order U^{-3}.

3. At the order 2, this last degeneracy is again partially lifted: both lines decompose into 4 lines which separate the domains where s^-, $-s_3$, $-s_2$, $-s_1$, s_{cb}, s_1, s_2, s_3, s^+ are g.s.c. On the lines which separate $(s^-, -s_3)$, $(-s_1, s_{cb})$, (s_{cb}, s_1), (s_3, s^+) the number of g.s.c. is infinite.

From this discussion we are led to conjecture that the phase diagram of the 2-dimensional Falicov–Kimball model will contain an infinite number of domains with a devil's-staircase structure similar to the one previously observed in 1 dimension.[6]

APPENDIX A

We give here a list of the various generalizations needed in order to extend the results of ref. 1, obtained by the moment method, to ν dimensions.

The moments $m_\mu(k, s)$ are given by the same formula as in ref. 1 with the following substitutions:

$$\mathbf{c}_1 = \begin{pmatrix} c_{1;1} \\ \vdots \\ c_{1;\nu} \end{pmatrix}, \qquad c_{1;j} = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} s_x s_{x+e_j}, \qquad c_1 = \nu^{-1} \sum_{j=1}^{\nu} c_{1;j} \tag{A1}$$

$$\mathbf{c}_2 = \begin{pmatrix} c_{2;(1,2,+)} \\ c_{2;(1,2,-)} \\ \vdots \\ c_{2;(\nu-1,\nu,-)} \end{pmatrix}, \qquad c_{2;(i,j,\pm)} = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} s_x s_{x+(e_i \pm e_j)} \tag{A2}$$

$$c_2 = [\nu(\nu-1)]^{-1} \sum_{i,j,\sigma} c_{2;(i,j,\sigma)}$$

$$\mathbf{c}_3 = \begin{pmatrix} c_{3;1} \\ \vdots \\ c_{3;\nu} \end{pmatrix}, \qquad c_{3;j} = \frac{1}{|\Lambda|} \sum_{x \in \Lambda} s_x s_{x+2e_j}, \qquad c_3 = \nu^{-1} \sum_{j} c_{3;j} \tag{A3}$$

$$\mathbf{A} = 2\begin{pmatrix} \cos k_1 \\ \vdots \\ \cos k_\nu \end{pmatrix}, \qquad A = 2\sum_{j=1}^{\nu} \cos k_j \tag{A4}$$

$$\mathbf{B} = \begin{pmatrix} \cos(k_1+k_2) \\ \cos(k_1-k_2) \\ \vdots \\ \cos(k_{\nu-1}-k_\nu) \end{pmatrix}, \qquad \mathbf{C} = 2\begin{pmatrix} \cos 2k_1 \\ \vdots \\ \cos 2k_\nu \end{pmatrix} \tag{A5}$$

In the vicinity of $s = s_{cb}$ we have the same relations between the correlations c_1, c_2, and c_3 as in two dimensions. For instance, we derive the relation 3 of ref. 7: for any i, j, $i \neq j$,

$$0 \leqslant 1 + \tfrac{1}{2}(c_{3;i} + c_{3;j}) - (c_{2;(i,j,+)} + c_{2;(i,j,-)})$$

Hence

$$\begin{aligned} 0 &\leqslant \sum_{i<j} [1 + \tfrac{1}{2}(c_{3;i} + c_{3;j}) - (c_{2;(i,j,+)} + c_{2;(i,j,-)})] \\ &= \nu(\nu-1)/2 + \nu(\nu-1)c_3/2 - \nu(\nu-1)c_2 \end{aligned}$$

i.e.,

$$1 + c_3 - 2c_2 \geqslant 0$$

APPENDIX B

Here we define the quantities that appeared in Properties 8 and 9. The function $f_+(\tilde{\mu}_e)$ that gives the boundary of the region where s^+ is the ground state has the form

$$\begin{aligned} f_+(\tilde{\mu}_e) = & -U + \frac{4U^2}{(2\pi)^\nu}(U + 2\nu + \tilde{\mu}_e)\int_{\mathscr{D}_1} d^\nu k\,(2U + 2\nu - A)^{-2} \\ & + \frac{U}{(2\pi)^\nu}\int_{\mathscr{D}_2} d^\nu k\,(A + \tilde{\mu}_e)\,|A - U + \tilde{\mu}_e|^{-1} \end{aligned} \tag{B1}$$

where

$$\mathscr{D}_1 = \{k \mid A(k) \leqslant 2\tilde{\mu}_e - 4\}, \qquad \mathscr{D}_2 = [0, 2\pi]^\nu \backslash \mathscr{D}_1$$

The parameters that enter into the linear functions that bound the region where s_{cb} are the g.s.c. are

$$C(U)=\frac{1}{(2\pi)^{\nu}}\int d^{\nu}k\,(1+A^{2}/U^{2})^{-3/2}\underset{U\to\infty}{\simeq}1-\frac{3\nu}{U^{2}}$$

$$D(U)=\frac{U^{2}}{(2\pi)^{\nu}}\int d^{\nu}k\,\frac{A^{2}(2\varepsilon+\gamma)}{\varepsilon^{3}(\varepsilon+\gamma)^{2}}\underset{U\to\infty}{\simeq}\frac{3\nu}{2U^{2}} \tag{B2}$$

$$b(U)=\frac{U^{2}}{(2\pi)^{\nu}}\int d^{\nu}k\,\frac{A^{2}}{\varepsilon(\varepsilon+\gamma)^{2}}\underset{U\to\infty}{\simeq}\frac{\nu}{2U}$$

where

$$\varepsilon=(A^{2}+U^{2})^{1/2},\qquad \gamma=U+2\nu$$

The parameter σ that specifies the interval of admissible values of $\tilde{\mu}_e$ is

$$\sigma=\frac{U}{3(1+2\nu/3U)}$$

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