Ground-state properties of multicomponent Falicov–Kimball-like models I

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Abstract

We consider a classical lattice gas that consists of more than one “species” of particles (like a spin-$\frac{3}{2}$ Ising model or the atomic limit of the extended Hubbard model), whose ground-state phase diagram is macroscopically degenerate. This gas is coupled component-wise and in the Falicov–Kimball-like manner to a multicomponent free-fermion gas. We show rigorously that a component-wise coupling of the classical subsystem to the quantum one orders the classical subsystem so that the macroscopic degeneracy is removed.

Key words: Fermion lattice systems, Ground-state phase diagrams, Strongly correlated electrons, Falicov–Kimball model, Extended Hubbard model

PACS: 71.10.-w, 71.27.+a

1 Introduction

The Hamiltonians of the so-called strongly correlated electron systems describe in fact multicomponent gases of quasiparticle excitations in a crystal. The components are labeled, by orbital and/or spin degrees of freedom, for instance. As a rule, revealing cooperative phenomena in such systems, like long-range orders, is a hard task. Then, in the course of studies, one simplifies the Hamiltonian by discarding some labels of quasiparticles, setting some coupling constants to zero and sending other to infinity. Simultaneously, one looses possibilities of accounting for some physics. But once a sufficient level

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of understanding of a simplified model is reached, a reverse process starts.
This might be a brief history of the Falicov–Kimball model (and only to some extent of the Hubbard model) studies.

The original model put forward by Falicov and Kimball [1,2] refers to two groups of quasiparticles excitations, called localized holes and itinerant electrons, with the members of each group labeled by band and spin indices. Only a few, out of many, on-site interactions of these quasiparticles are retained and the strength of the on-site hole–hole repulsion is sent to infinity [2]. The extreme simplification of this model, that consists of one band of spinless electrons and of spinless holes, is known as the spinless Falicov–Kimball model. In contradistinction to the case of Hubbard model, it has been possible to demonstrate, without uncontrollable approximations, that the spinless Falicov–Kimball model exhibits a staggered long-range order [3,4,5]. Subsequent research extended considerably this result and supplied us with a fairly broad knowledge of the phase diagram. Naturally, the strongest results have been obtained at zero temperature (see [6,7] for more details and an extensive list of references).

Then, one observes a resurgence of interest in effects of additional degrees of freedom and additional interactions between localized particles. Most attention has been paid to effects related to spin degrees of freedom. Thus models, where the localized and intinerant quasiparticles carry spin-$\frac{1}{2}$ [8,9,10,11,12,13] have been investigated. In [8,9,13] a finite repulsion between localized particles with opposite spins has been included. Quite recently, it was argued that an interesting physics could be accounted for by multicomponent Falicov–Kimball models [14]. As a preliminary step, a kind of Falicov–Kimball model with $2s + 1$ components of itinerant particles and $2S + 1$ components of localized ones was solved exactly in the limit of infinite dimensions. Concerning interactions between localized particles, only an on-site repulsion between different components of localized particles was included and its strength was sent to infinity, thereby restricting the space of states available for the system. Unlike in the quoted above papers on the spin-$\frac{1}{2}$ case, $s$ may not be equal to $S$.

The multicomponent Falicov–Kimball models, we referred to above, belong to a class of systems whose generic Hamiltonian is of the form

$$H_\Lambda = \sum_\sigma T_\sigma + \sum_{x,\sigma,\eta} U_{\sigma\eta} n^e_{x,\sigma} n^i_{x,\eta} + H_i.$$  \hspace{1cm} (1)

The first sum, over $\sigma$-components of itinerant fermions (later on called briefly electrons), accounts for their hopping. The second sum, over lattice sites $x$, $\sigma$-components of electrons and $\eta$-components of localized particles (later on called ions), represents the usual Falicov–Kimball-like coupling between the itinerant and localized particles. With $n^e_{x,\sigma}$, $n^i_{x,\eta}$ being the occupation number
operators at site \( x \) of \( \sigma \)-electrons and \( \eta \)-ions, respectively, it contributes the energy \( U_{\sigma\eta} \) if and only if the site \( x \) is occupied by a \( \sigma \)-electron and an \( \eta \)-ion. The third term, \( H_i \), stands for an interaction between ions, diagonal in their occupation-number representation. Therefore, the system described by the Hamiltonian \( H_\Lambda \) can be looked upon as a multicomponent classical gas (of ions) coupled to a multicomponent free-fermion gas (of electrons).

In the main body of this paper we study an instance of (1) with a component-wise coupling between the electrons and ions, i.e., we set \( U_{\sigma\eta} = U_{\sigma}\delta_{\sigma\eta} \). The component-wise coupling may appear naturally in situations, where the components differ significantly in their physical characteristics. Actually, we make the coupling component-independent, \( U_{\sigma} = U \) for all \( \sigma \), and assume equal number of electrons’ and ions’ components, for simplicity. If \( H_i \) involves only finite-range interactions that admit a representation in terms of a m-potential [15], then some aspects of the ground state of the model, defined by \( H_\Lambda \), concerned with the distribution of ions on the underlying lattice, can readily be investigated by the methods developed in [4,16].

However, if the itinerant and localized particles are interpreted as different sorts of electrons, as is the case in the original paper by Falicov and Kimball, and the coupling between electrons stands for a screened Coulomb repulsion, then an ion-independent coupling, i.e., \( U_{\sigma\eta} = U_{\sigma} \), becomes more appropriate. Such a coupling has been studied rigorously in [8,9] and in the limit of infinite dimensions in [14]. The multicomponent Falicov–Kimball models with ion-independent coupling will be the subject of our subsequent paper.

In the next section we provide necessary details and properties of our model with the component-wise coupling, as well as definitions useful in considerations of ground-state phase diagrams in the grand-canonical ensemble. Then, in Section 3 we study the ground-state phase diagram at the hole–particle symmetry point in the plane of chemical potentials of electrons and ions, for arbitrary strength \( U \) of the electron–ion coupling. After that, in Section 4 we go beyond the hole–particle symmetry point, but only in the strong-coupling regime. Finally, in Section 5, we provide a summary and discussion of the obtained results.

2 The model and the grand canonical ground states

In the sequel we study a version of the model (1) specified as follows. The underlying finite lattice \( \Lambda \), consisting of \( |\Lambda| \) sites, is assumed to be a piece of a \( d \)-dimensional hypercubic lattice \( \mathbb{Z}^d \), such that it can be partitioned into two congruent sublattices: the even sublattice, \( \Lambda^e \), and the odd sublattice, \( \Lambda^o \). Each site of \( \Lambda \) has \( z = 2d \) nearest neighbours. Then, the nearest-neighbour
sites of a site in $\Lambda^e$ belong to $\Lambda^o$ and vice versa. We shall use the notation $\langle x, y \rangle \equiv \langle x, y \rangle_1, \langle x, y \rangle_i, \ i = 1, 2, \ldots, \ x, y \in \Lambda, to$ denote the first and the $i$-th nearest neighbours on $\Lambda$, that is the unordered pairs of sites whose Euclidean distance in the units of the lattice constant are $1, \sqrt{2}, 2, \ldots, \ for \ i = 1, 2, 3, \ldots,$ respectively. Consequently, $\sum_{\langle x, y \rangle_i}$ will stand for the summation over all the $i$-th nearest-neighbour pairs of sites, with each pair counted once.

The quantum subsystem, consisting of $r \geq 2$ different kinds of itinerant particles (electrons) labelled by $\sigma = 1, 2, \ldots, r$, is described in terms of creation and annihilation operators of a $\sigma$-electron at site $x \in \Lambda$: $c_{x, \sigma}^+, c_{x, \sigma}$, respectively. The operators $\{c_{x, \sigma}^+, c_{x, \sigma}\}_{x \in \Lambda}^{\sigma=1,\ldots,r}$ satisfy the canonical anticommutation relations. Then, the hopping of $\sigma$-electrons is specified by:

$$T_\sigma = t \sum_{\langle x, y \rangle} \left( c_{x, \sigma}^+ c_{y, \sigma} + h.c. \right),$$

with $t$ being the nearest-neighbour hopping intensity. Another relevant observable is the total electron-number operator $N_e = \sum_\sigma N_{e, \sigma}$, where $\sigma$-electron-number operators $N_{e, \sigma} = \sum_x n_{e, x, \sigma}$ and $n_{e, x, \sigma} = c_{x, \sigma}^+ c_{x, \sigma}$.

The classical subsystem consists also of $r \geq 2$ different kinds of particles (localized ions). The states of this subsystem can be described by a collection of particle-occupation numbers $C = \{n_{i, x, \sigma}^i\}_{x \in \Lambda}^{\sigma=1,\ldots,r}$, with $n_{i, x, \sigma}^i = 0, 1$ (no two ions occupying the same site can be of the same kind), called the ion configurations. The total number of ions is $N_i = \sum_\sigma N_{i, \sigma}$, where the numbers of $\sigma$-ions $N_{i, \sigma} = \sum_x n_{i, x, \sigma}^i$. In contradistinction to the electron subsystem, we introduce a direct ion-ion interaction. Each pair of ions occupying a site contributes the energy $2I$. Moreover, two ions that occupy two nearest-neighbour sites repel each other, contributing the energy $W/2 > 0$. Thus, the ion–ion interaction Hamiltonian, $H_i$, reads

$$H_i = 2I \sum_{\sigma' < \sigma''} \sum_x n_{x, \sigma'}^i n_{x, \sigma''}^i + \frac{W}{2} \sum_{\langle x, y \rangle} n_{x}^i n_{y}^i,$$

where $n_x^i = \sum_\sigma n_{x, \sigma}^i$ and $\sum_{\sigma' < \sigma''}$ stands for the summation over unordered pairs of indices $(\sigma', \sigma'')$, each pair being counted once.

Clearly, in the composite system, whose Hamiltonian is given by (1), (2) and (3) (with arbitrary matrix $U_{\sigma\eta}$), the particle-number operators $N_{e, \sigma}$ (hence $N_e$) are conserved. The peculiarity of this system is that the site-occupation numbers $n_{i, x, \sigma}^i$ (hence $N_{i, \sigma}$ and $N_i$) are also conserved and therefore the description of the classical subsystem in terms of the ion configurations $C = \{n_{i, x, \sigma}^i\}_{x \in \Lambda}^{\sigma=1,\ldots,r}$ remains valid.
Finally, the coupling between the classical and quantum subsystems is chosen to be the component-wise one, with

\[ U_{\sigma \eta} = 2U \delta_{\sigma \eta}. \]  

(4)

This concludes the specification of our system.

In what follows, we shall study the ground-state phase diagram of the system defined by (1)–(4), in the grand canonical ensemble. Ultimately, this task amounts to determining at each point \((\tilde{\mu}_e, \tilde{\mu}_i)\) of the plane of chemical potentials of electrons and ions, respectively, the lowest energy eigensubspace of the Hamiltonian

\[ \tilde{H}_\Lambda (\tilde{\mu}_e, \tilde{\mu}_i) = H_\Lambda - \tilde{\mu}_e N_e - \tilde{\mu}_i N_i. \]

(5)

Actually, our purposes will be more restricted. Namely, we shall be interested only in determining the set of periodic ground-state configurations of ions at each point in the \((\tilde{\mu}_e, \tilde{\mu}_i)\) plane.

In studies of grand-canonical phase diagrams an important role is played by unitary transformations that exchange particles and holes: \(n_{x,\sigma}^e \rightarrow 1 - n_{x,\sigma}^e\) and \(n_{x,\sigma}^i \rightarrow 1 - n_{x,\sigma}^i\), and for some \((\tilde{\mu}_e^0, \tilde{\mu}_i^0)\) leave the Hamiltonian \(\tilde{H}_\Lambda (\tilde{\mu}_e, \tilde{\mu}_i)\) invariant. For the electron subsystem of (5) such a role is played by the transformations: \(c_{x,\sigma}^e \rightarrow (-1)^{|x|} c_{x,\sigma}\), with \(|x| = |(x_1, \ldots, x_d)| = \sum_{i=1}^d |x_i|\). At the hole–particle symmetry point, \((\tilde{\mu}_e^0, \tilde{\mu}_i^0)\), the system under consideration has very special properties, which facilitate studies of its phase diagram (among them is the property that the grand-canonical expectations of \(n_{x,\sigma}^e, n_{x,\sigma}^i\) assume the value of \(1/2\), independently of temperature). One easily finds that this system is hole–particle invariant at the point \((\tilde{\mu}_e^0, \tilde{\mu}_i^0)\), where

\[ \tilde{\mu}_e^0 = U, \quad \tilde{\mu}_i^0 = \tilde{\nu}_i^0 + U, \quad \tilde{\nu}_i^0 = \frac{W}{4} rz + I(r - 1). \]

For future purposes, it is convenient to introduce the shifted chemical potentials

\[ \mu_e = \tilde{\mu}_e - \tilde{\mu}_e^0, \quad \mu_i = \tilde{\mu}_i - \tilde{\mu}_i^0, \]

the new Hamiltonian \(H_\Lambda (\mu_e, \mu_i) = \tilde{H}_\Lambda (\tilde{\mu}_e, \tilde{\mu}_i)\), and express \(H_\Lambda (\mu_e, \mu_i)\) as follows

\[ H_\Lambda (\mu_e, \mu_i) = \sum_\sigma \left( H_{\sigma}^{FK} - \mu_e N_{e,\sigma} - \mu_i N_{i,\sigma} \right) + H_i^0, \]  

(6)
\[ H_{FK} = T + 2U \sum_x n^e_{x,\sigma} n^i_{x,\sigma} - UN_{e,\sigma} - UN_{i,\sigma} \]
\[ = T + 2U \sum_x \left( n^e_{x,\sigma} - \frac{1}{2} \right) \left( n^i_{x,\sigma} - \frac{1}{2} \right), \quad (7) \]
\[ H_0^i = H_i - \tilde{v}^0_i N_i \]
\[ = 2I \sum_{x,\sigma' < \sigma''} \left( n^i_{x,\sigma'} - \frac{1}{2} \right) \left( n^i_{x,\sigma''} - \frac{1}{2} \right) + \frac{W}{2} \sum_{\langle x,y \rangle} \left( n^i_x - \frac{r}{2} \right) \left( n^i_y - \frac{r}{2} \right). \quad (8) \]

The second equalities in (7, 8) hold up to a term which is independent of the particle states. The Hamiltonians \( H_{FK} \) and \( H_0^i \) are invariant with respect to the hole–particle transformation, consequently \( H_{\Lambda}(\mu_e, \mu_i) \) is hole–particle invariant at the point \( \mu_e = \mu_i = 0 \).

We define \( E_C(\mu_e, \mu_i) \) to be the ground-state energy of \( H_{\Lambda}(\mu_e, \mu_i) \) for a given configuration of ions \( C \). Then the ground-state energy of the Hamiltonian \( H_{\Lambda}(\mu_e, \mu_i) \), denoted \( E_G(\mu_e, \mu_i) \), is \( E_G(\mu_e, \mu_i) = \min \{ E_C(\mu_e, \mu_i) : C \} \), and the minimum is attained at the set \( G \) of the ground-state configurations of ions.

### 3 Ground-state phase diagram at the hole–particle symmetry point

In this section we shall describe the ground-state configurations of ions in the systems given by \( H_0^i \) and \( H_{\Lambda}(0,0) \).

Let us consider first the classical subsystem of ions, given by \( H_0^i \). The nature of its ground-state configurations of ions is explained by the Theorem 1, which follows. Briefly, there are two domains of couplings \( I, W \), differentiated by the ratio \( \delta = 4I/zW \). For \( \delta < 1 \), there are exactly two ground-state configurations, while for \( \delta \geq 1 \) there is a macroscopic degeneracy (i.e., the number of ground-state configurations grows exponentially with the size \( |\Lambda| \) of the underlying lattice).

**Theorem 1** Consider the system given by \( H_0^i \), with \( W > 0 \).

(i) If \( 4I < zW \), the set of ground-state configurations consists of exactly two ion configurations with the following property: each site of one of the sublattices of \( \Lambda \) is occupied by \( r \) ions while the complementary sublattice is empty.

(ii) If \( 4I > zW \), the set of ground-state configurations contains macroscopically many elements.

For even \( r \), \( r = 2k \), any ion configuration with \( k \) ions in each site is the ground-state one; the degeneracy of the ground state is \( (C_r^k)^{|\Lambda|} \), where \( C_r^k = \)}
For odd $r$, $r = 2k+1$, any ion configuration satisfying the condition: each site of one sublattice is occupied by $k$ ions while each site of the complementary sublattice by $(k+1)$ ions, is the ground-state configuration; the degeneracy is $(C_r^k)^{|\Lambda|/2}(C_r^{(k+1)})^{|\Lambda|/2}$.

(iii) If $4I = zW$ the set of ground-state configurations contains macroscopically many elements: any configuration of kind (i) or (ii) is the ground-state configuration.

A proof of Theorem 1 is given in appendix.

Now, consider the composite system that consists of $r$ components of classical ions coupled to $r$ components of quantum electrons, described by the Hamiltonian $H_\Lambda(0,0)$. The following theorem characterizes the ground-state configurations of ions at the hole–particle symmetry point.

**Theorem 2** Consider the system given by $H_\Lambda(0,0)$ with $U \neq 0$ and $W > 0$.

(i) If $4I < zW$, then the ground-state energy is attained for exactly two ion configurations that satisfy the following condition. The ions fill out completely one sublattice of $\Lambda$, i.e., each site of this sublattice is occupied by $r$ ions, while the complementary sublattice is empty.

(ii) If $4I > zW$, then the set of ground-state configurations of ions contains finitely many elements; any two nearest-neighbour sites cannot be occupied by ions of the same kind.

Moreover, for $r$ even, $r = 2k$, there are exactly $C_r^k$ ground-state configurations of ions; each site of $\Lambda$ is occupied by $k$ ions.

For $r$ odd, $r = 2k + 1$, there are exactly $2C_r^k$ ground-state configurations of ions with the following property: each site of one sublattice is occupied by $k$ ions, while each site of the complementary sublattice contains $k + 1$ ions.

(iii) If $4I = zW$, the set of ground-state configurations of ions consists of finitely many elements: any configuration of kind (i) or (ii) is the ground-state configuration.

Thus, the effect of the component-wise coupling of our classical gas of ions with quantum electrons amounts to removing the macroscopic degeneracy of the domain of $I, W$, where $\delta \geq 1$. The domain, where $\delta < 1$, of finite degeneracy is left unchanged. This effect does not depend neither on the hopping intensity $t$ nor on the strength $U$ of the ion-electron coupling.

To prove the Theorem 2, let us note that since the operators $H_{\sigma FK}^\sigma$ ($\sigma = 1, \ldots, r$), $H_{i}^0$, commute pairwise, for given configuration $C$

$$E_C(0,0) = \sum_\sigma E_{C_\sigma}^{FK} + E_C^i,$$

where $E_{C_\sigma}^{FK}$ is the ground-state energy of $H_{\sigma FK}^\sigma$ for the configuration $C_\sigma =$
\[{n^i_{x,\sigma}}\}_{x \in \Lambda}\) that is the restriction of \(C\) to \(\sigma\)-ions, and \(E^i_{C}\) is the value of \(H^0_i\) at \(C\). Let \(E^F_{G}\) be the ground-state energy of \(H^F_{\sigma}\), i.e. \(E^F_G = \min \{E^F_{C_\sigma} : C_\sigma\}\) and the minimum is attained at the configurations \(C_\sigma \in G^F_{\sigma}\). The energy \(E^F_G\) and the set \(G^F_{\sigma}\) do not depend on \(\sigma\). Let \(E^i_{C_\sigma}\) be the value of \(H^0_i\) at \(C_\sigma\). Let \(E^F_{G}\) and the set \(G^F_{\sigma}\) do not depend on \(\sigma\). Let \(E^i_G = \min \{E^i_C : C\}\) and let \(G^i\) be the set of configurations for which the minimum is attained. In general

\[E_G(0, 0) \geq \sum_\sigma E^F_{G_\sigma} + E^i_G. \quad (10)\]

However, we shall show that the lower bound (10) of \(E^F_G\) is attained for the set \(G\) of the configurations described in Theorem 2.

Consider first the term \(\sum_\sigma E^F_{C_\sigma}\) of (9). Clearly,

\[\min \left\{\sum_\sigma E^F_{C_\sigma} : C = (C_1, \ldots, C_r)\right\} = rE^F_G\]

and is attained for configurations in

\[G^F = \{(C_1, \ldots, C_r) : C_\sigma \in G^F_{\sigma}, \sigma = 1, \ldots, r\}\].

In order to determine \(G^F_{\sigma}\) (and \(E^F_G\)) we follow [4]. Note that, for a fixed configuration \(C\) the operator \(H^F_{\sigma} + U \sum_x \left(n^i_{x,\sigma} - \frac{1}{2}\right)\) is the second quantized form of the one-particle operator \(h_\sigma = T + US_\sigma\), where \(T\) and \(S_\sigma\) are \(|\Lambda| \times |\Lambda|\) matrices with the following matrix elements \([T]_{xy}, [S_\sigma]_{xy}\):

\[ [T]_{xy} = \begin{cases} t, & \text{if } x, y \text{ are nearest neighbours on } \Lambda \\ 0, & \text{otherwise} \end{cases} \]

\[ [S_\sigma]_{xy} = s_{x,\sigma} \delta_{xy}, \quad s_{x,\sigma} = 2n^i_{x,\sigma} - 1. \]

The lowest eigenvalue of \(H^F_{\sigma} + U \sum_x \left(n^i_{x,\sigma} - \frac{1}{2}\right)\) is the Fermi-sea energy of \(h_\sigma\) corresponding to the Fermi level \(\mu_e = 0\). Thus, in terms of the eigenvalues \(\lambda^i_j, j = 1, \ldots, |\Lambda|\), of the operator \(h_\sigma\)

\[E^F_{C_\sigma} = \sum_{\lambda^i_j < 0} \lambda^i_j - \frac{U}{2} \sum_x s_{x,\sigma} = -\frac{1}{2} \left[ \sum_{\lambda^i_j} |\lambda^i_j| - \sum_{\lambda^i_j} \lambda^i_j \right] - \frac{U}{2} \sum_x s_{x,\sigma} = -\frac{1}{2} \text{Tr}[h_\sigma] - \text{Tr}[h_\sigma] - \frac{U}{2} \sum_x s_{x,\sigma} = -\frac{1}{2} \text{Tr}[h_\sigma], \]

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since $\text{Tr} T = 0$. Kennedy and Lieb have proved in [4] that

$$-\text{Tr}|h_\sigma| \geq -\text{Tr}(T^2 + U^2)$$

and the lower bound is attained for exactly two configurations $C_\sigma$ with the following property: one sublattice of $\Lambda$ is completely occupied by $\sigma$-ions while the complementary sublattice is empty. Thus, $E^{FK}_G = -\frac{1}{2}\text{Tr}(T^2 + U^2)$ and the described above configurations constitute $G^{FK}_\sigma$.

The set $G^i$ is specified in Theorem 1. Now, since $G^{FK} \cap G^i$ is nonvoid, the set $G$ of ground-state configurations of $H_\Lambda(0,0)$ is $G = G^{FK} \cap G^i$ and the ground-state energy equals to $E_G(0,0) = -\frac{1}{2}\text{Tr}(T^2 + U^2) + E^i_G$.

In the following section we shall show that the effect of removing macroscopic degeneracies of classical-ion phases persists off the hole–particle symmetry point.

4 Ground states off the symmetry point in the strong-coupling regime

Let us consider the system given by (6), (7) and (8) with $\mu_i \neq 0$. In order to simplify the arguments that follow, we set $r = 2$, with the label $\sigma$ interpreted as spin-$\frac{1}{2}$ and taking values in $\{\uparrow, \downarrow\}$. Moreover, the calculations are carried out for $d = 2$, i.e. $\Lambda$ is a piece of the square lattice, but the obtained results can be generalized to higher-dimensional hypercubic lattices in a straightforward way.

As in the previous section, we start with the classical subsystem whose Hamiltonian is $H^0_\Lambda - \mu_i N_i$, and is specified by (8). The ground-state phase diagram in the plane $(I/W, \mu_i/W)$ can be obtained by extending the calculations of Appendix A, and is shown in Fig. 1.

The energies of ion configurations depend only on the occupation numbers of sites: $n^i_x = 2, 1, 0$. Consequently, the ground-state configurations in the domains $B, C_+, C_-$ are macroscopically degenerate due to the spin degeneracy.

According to the Theorem 2, at the line $\mu_i = 0$ and in the domain $B$, the coupling to the electron subsystem orders the ion subsystem antiferromagnetically: each sublattice is occupied exclusively by one kind of ions.

In order to determine the effect on the macroscopically degenerate ground-state configurations of the coupling to the electron subsystem, off the line $\mu_i = 0$, we resort to the strong-coupling limit. In this limit, the two components
Fig. 1. Ground-state phase diagram of $H_i^0 - \mu N_i$, for $\mu \geq 0$. The ground-state configurations inside the regions $A$, $B$, $C_+$, $D_+$ are obtained by periodizing the elementary-plaquette configurations displayed inside the regions $A$, $D_+$ and those located by the starting points of the arrows in $B$, $C_+$. The elementary-plaquette configurations located by the end points of the arrows in $B$, $C_+$ show the effect of the coupling to the electron subsystem. The second half of the diagram, for $\mu < 0$, containing the second halves of the regions $A$, $B$ and the regions $C_-$, $D_-$, can be obtained by reflecting the part with $\mu > 0$ in the line $\mu = 0$ and simultaneously replacing the elementary-plaquette configurations, by their hole–particle counterparts ($n^i_x \to 2 - n^i_x$).

$H_{\sigma} - \mu_e N_{e,\sigma}$ of $H_{\Lambda}(\mu_e, \mu_i)$ can be expanded into a power series in $1/|U|$ [16]. The obtained series is convergent absolutely and uniformly in $|\Lambda|$, provided $|U| > zt$ and $|\mu_e| < |U| - zt$ (here $z = 4$) [17,18]. Due to symmetries of $H_{\Lambda}(\mu_e, \mu_i)$ we can restrict our considerations to the case $U > 0$, and set $N_{e,\sigma} = |\Lambda| - N_{i,\sigma}$ [4,16].

Let $H_{\Lambda}^{(k)}(\mu_e, \mu_i)$, $k = 1, 2, \ldots$, stand for the partial sums of the $1/U$ expansion of $H_{\Lambda}(\mu_e, \mu_i)$. Then, up to a term independent of the ion configurations, the partial sum $H_{\Lambda}^{(3)}(\mu_e, \mu_i)$ reads [16]:

\[
H_{\Lambda}^{(3)}(\mu_e, \mu_i) = -\frac{\mu_i}{2} \sum_x (s_{x,\uparrow} + s_{x,\downarrow}) + \frac{I}{2} \sum_x s_{x,\uparrow}s_{x,\downarrow} + \frac{W}{8} \sum_{\langle x,y \rangle_1} (s_{x,\uparrow} + s_{x,\downarrow})(s_{y,\uparrow} + s_{y,\downarrow})
\]

\[
+ \left( \frac{t^2}{4U} - \frac{9t^4}{16U^3} \right) \sum_{\langle x,y \rangle_1} (s_{x,\uparrow}s_{y,\uparrow} + s_{x,\downarrow}s_{y,\downarrow}) + \frac{3t^4}{16U^3} \sum_{\langle x,y \rangle_2} (s_{x,\uparrow}s_{y,\uparrow} + s_{x,\downarrow}s_{y,\downarrow}) + \frac{t^4}{8U^3} \sum_{\langle x,y \rangle_3} (s_{x,\uparrow}s_{y,\uparrow} + s_{x,\downarrow}s_{y,\downarrow})
\]
\[ + \frac{5t^4}{16U^3} \sum_{p} (s_{x,\uparrow}s_{y,\uparrow}s_{z,\uparrow}s_{w,\uparrow} + s_{x,\downarrow}s_{y,\downarrow}s_{z,\downarrow}s_{w,\downarrow}) + O \left( \frac{t^6}{U^5} \right). \]  \hspace{1cm} (11)

Since \( H^{(0)}_{\Lambda}(\mu_e, \mu_i) \) differs from \( H^0_i - \mu_i N_i \) by a constant, at the zero order the phase diagram coincides with that of the classical subsystem. In the first order, \( H^{(0)}_{\Lambda}(\mu_e, \mu_i) \) is augmented by the Ising antiferromagnetic interaction of the strength \( t^2/4U \). Consequently, in the phase diagram of \( H^{(1)}_{\Lambda}(\mu_e, \mu_i) \) the domains \( B, C_+, C_- \) are replaced by some domains \( B^{(1)}, C^{(1)}_+, C^{(1)}_- \), whose boundaries are shifted with respect to the boundaries of \( B, C_+, C_- \) by terms of the order \( 1/U \). The set of ground-state configurations inside \( B^{(1)} \) consists only of the two antiferromagnetic configurations, while the sets of ground-state configurations inside \( C^{(1)}_+, C^{(1)}_- \) remain the same as those in \( C_+, C_- \). Passing to the next order, one finds that the phase diagram of \( H^{(3)}_{\Lambda}(\mu_e, \mu_i) \) contains some domains \( B^{(3)}, C^{(3)}_+, C^{(3)}_- \) whose boundaries are shifted with respect to the boundaries of domains \( B^{(1)}, C^{(1)}_+, C^{(1)}_- \) by terms of the order \( 1/U^3 \). In this order, the set of ground-state configurations inside \( B^{(3)} \) remains the same as that in \( B^{(1)} \). On the other hand, the macroscopically degenerate sets of ground-state configurations in \( C^{(1)}_+ \) \( (C^{(1)}_-) \) are replaced by exactly four configurations in \( C^{(3)}_+ \) \( (C^{(3)}_-) \): one sublattice is doubly occupied (empty) while the complementary sublattice is ordered antiferromagnetically. Applying the arguments due to Kennedy [17] and Gruber et al. [18], we conclude that there are nonvoid domains \( B^{(\infty)}, C^{(\infty)}_+, C^{(\infty)}_- \) such that \( B^{(\infty)} \subset B^{(3)} \), \( C^{(\infty)}_+ \subset C^{(3)}_+ \), \( C^{(\infty)}_- \subset C^{(3)}_- \), inside which the sets of ground-state configurations of \( H_{\Lambda}(\mu_e, \mu_i) \) coincide with those inside \( B^{(3)}, C^{(3)}_+, C^{(3)}_- \), respectively.

5 Discussion

The two-component classical system considered in Section 4 and given by the Hamiltonian \( H^0_i - \mu_i N_i \) is well known in the literature of strongly correlated electron systems as the atomic limit of the extended Hubbard model. A lot of effort has been devoted to studies of its phase diagram, see for instance [19,20] and references quoted there. When the two kinds of ions involved (in the context of Hubbard-like models they are interpreted as localized electrons with spin up or down) are allowed to hop, we arrive at the extended Hubbard model. This model is, since many years, a subject of vigorous research. One of the intriguing questions asked is what is the effect of hopping on the phases of localized electrons (determined in the atomic limit). It is widely known that the second-order perturbation theory, with respect to hopping, predicts that the ground-state configurations with only singly occupied sites (inside domain \( B \)) are ordered antiferromagnetically by a weak hopping, Brandt and
Stolze have shown [21] that the prediction for the phase with density \( \frac{1}{2} \left( \frac{1}{2} \right) \), inside domain \( C_+ (C_-) \), is that it is ordered ferromagnetically by a weak hopping, what results in coexistence of charge and magnetic orders. Thus, according to the second-order perturbation theory the quantum fluctuations, introduced by the hopping, remove the spin degeneracy present in the ground-state phases of localized electrons. In this paper we address an analogous problem. In our case however, the direct quantum fluctuations introduced by the hopping of the ions are replaced by the indirect ones, introduced by the hopping of an extra quantum system of free electrons coupled to the classical system of ions in a Falicov–Kimball way. In this new set up, the effect of quantum fluctuations due to the hopping could have been studied rigorously. In Section 3, we have considered only the hole–particle symmetry point. For any strength of the coupling between electrons and ions and any hopping, we obtained that the ground-state configurations of singly occupied sites (when there is no hopping of electrons), become antiferromagnetically ordered upon switching the hopping. This result agrees with the predictions of the perturbation theory for the extended Hubbard model. However, far away of the symmetry point, inside the domains \( C_+ (C_-) \), where without hopping the ground-state configurations are spin degenerate, we also find an antiferromagnetic order upon switching the hopping. This result is in contrast with the predictions of the perturbation theory for the extended Hubbard model.

Acknowledgements

One of the authors (V.D.) is grateful to the University of Wroclaw, and especially to the Institute of Theoretical Physics for financial support.

Appendix

In order to prove Theorem 1, it is enough to notice that if \( Q_x = n^1_x - r/2 \), then (8) reads:

\[
H^0_i = \frac{W}{4} \sum_{(x,y)} (Q_x + Q_y)^2 - \left( \frac{W}{4} z - I \right) \sum_x Q^2_x.
\]

Rewriting \( H^0_i \) in terms of a nearest-neighbour bond potential \( \phi_{(x,y)} \):

\[
H^0_i = \sum_{(x,y)} \phi_{(x,y)},
\]
\[
\phi(x,y) = \frac{W}{4}(Q_x + Q_y)^2 - \left(\frac{W}{4} - \frac{I}{z}\right)(Q_x^2 + Q_y^2),
\]

and minimizing \(\phi(x,y)\) one finds that it is a m-potential, which gives us the periodic ground-state configurations of \(H_0^i\). The set \(G_i\) of configurations which realize the minimum of the energy \(E_i^C\) \((W > 0)\), in the terms of \(Q_x\), consists of configurations whose restriction to the nearest-neighbour bonds \(\langle x, y \rangle\) is as follows:

a) \(r = 2k, 4I > zW\), \((Q_x, Q_y) = (0, 0)\),
b) \(r = 2k, 4I < zW\), \((Q_x, Q_y) = (-k, k)\),
c) \(r = 2k + 1, 4I > zW\), \((Q_x, Q_y) = (-1/2, 1/2)\),
d) \(r = 2k + 1, 4I < zW\), \((Q_x, Q_y) = (-k - 1/2, k + 1/2)\);

or in terms of \(n_x^i\)

a) \(4I > zW\), \(r = 2k + 1\), \((n_x^i, n_y^i) = (k, k + 1)\),
b) \(4I > zW\), \(r = 2k\), \((n_x^i, n_y^i) = (k, k)\)
c) \(4I < zW\), \((n_x^i, n_y^i) = (r, 0)\).

Periodizing these bond configurations one obtains \(G_i\).

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