Journal of Statistical Physics, Vol. 112, Nos. 5/6, September 2003 (© 2003)

Stability of Ground States of 2d Strongly Asymmetric Correlated-Hopping Hubbard Model

Jacek Wojtkiewicz[1]

Received October 7, 2002; accepted March 11, 2003

The asymmetric correlated-hopping Hubbard model is analysed perturbatively for large values of the Coulomb interaction U. An effective Hamiltonian is obtained up to terms of the order U^{-3}. For $d=2$ and in the limit of the strong asymmetry, the orderings of the ground states are found (confirming earlier nonrigorous results). Their thermal and quantum stability is proved. These results have been obtained by an application of the quantum Pirogov–Sinai theory in the variant developed by Datta, Fernandez, Fröhlich, and Rey-Bellet.

KEY WORDS: Falicov–Kimball model; Hubbard model; perturbation expansions; phase diagrams; Pirogov–Sinai theory.

1. INTRODUCTION

The model considered in this paper is an *asymmetric correlated-hopping Hubbard model* in a suitable range of parameters, described below. In this model, spin one-half electrons hop on the sites of a lattice Λ (assumed here as a subset of $\mathbb{Z}^d$) and interact only when they are on the same site.

The Hamiltonian defined on a finite subset Λ of $\mathbb{Z}^d$ has the form

$$H_\Lambda = H_{0,\Lambda} + V_\Lambda, \tag{1}$$

where

$$H_{0,\Lambda} = \sum_{i \in \Lambda} (U n_{i,+} n_{i,-} - \mu_+ n_{i,+} - \mu_- n_{i,-}) \tag{2}$$

$$V_\Lambda = -\sum_{\langle ij \rangle;\, \sigma} [t_\sigma + a_\sigma (n_{i,-\sigma} + n_{j,-\sigma})](c^\dagger_{i,\sigma} c_{j,\sigma} + c^\dagger_{j,\sigma} c_{i,\sigma}). \tag{3}$$

[1] Department for Mathematical Methods in Physics, Hoża 74, 00-682 Warsaw, Poland; e-mail: wjacek@fuw.edu.pl

0022-4715/03/0900-1127/0 © 2003 Plenum Publishing Corporation

Here $c^{\dagger}_{i,\sigma}$ and $c_{i,\sigma}$ are creation and annihilation operators of an electron of spin σ at lattice site $i \in \Lambda$, satisfying ordinary anticommutation relations. The corresponding particle number operator is $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$. The chemical potentials of electrons are μ_σ. The symbol $\langle ij \rangle$ denotes an orderless pair of nearest neighbour sites of the lattice. The constant U measures strength of the on-site Coulomb interaction; we assume that U is positive. Parameters t_σ are *hopping constants* (assumed to be positive) and a_σ describe *correlated hopping*.

There are important particular cases of the model characterized by the Hamiltonian above. The most famous case is the *Hubbard model* (HuM),[1,2] where $t_+ = t_-$, $a_\sigma = 0$. However, rigorous results concerning this model still are rare. The HuM belongs to the class of "notoriously difficult" models in E. Lieb' terminology.[3]

A much more tractable model is so called Falicov–Kimball (FKM) one; it corresponds to $t_+ = 0$, $t_- = t$, $a_\sigma = 0$. In this model, only one sort (say, "$-$") of particles hops, whereas the "$+$" particles are considered as classical ones. The FKM has been proposed in ref. 4 to description of the metal-insulator transition. Later, this model and its extensions have been applied to other situations: as a mathematical simplification of the Hubbard model; as a toy model of crystalization; to explain properties of mixed-valence compounds; to describe Peierls instability and Kondo effect. For excellent reviews, see refs. 5 and 6. In particular, one can hope that a good understanding of this simpler model might lead to better insight into the Hubbard model.[7]

The FKM attracts considerable attention, because it is one of the simplest quantum lattice models—it is highly non-trivial being however still tractable. There exist quite a large collection of rigorous results[5,6,8–12] which concern mainly the ground states structure and (in some cases) low-temperature properties.

The *asymmetric Hubbard model* is a model which "interpolates" between two limiting cases above (HuM and FKM); here, hopping constants have arbitrary spin-dependent values (values of a_σ are still set to 0). Some authors[7] say that "this interpretation is more convenient than physical." However, it seems that there is also strictly physical justification of this model, because one can find situation where some objects such as an *effective mass* (closely related to hopping constants) are explicitly spin-dependent—see ref. 13 and references therein.

After original versions of FKM (HuM) have been postulated, also their extensions and generalizations were considered. One of them is inclusion of the *correlated hopping term*, called also *bond-charge interaction*. Physically, presence of such term means that the hopping constant between given two sites depends of their occupation. Justification and importance of

such term have been stressed by numerous authors, both in the context of Hubbard model[1, 14, 16] as well as the FK one.[15] Again, one can give the "interpolating" version, and one obtains the model described by (2) and (3); it is an *asymmetric correlated-hopping Hubbard model* (aschHuM).

This paper is devoted to *strongly asymmetric correlated-hopping Hubbard model in a perturbative regime*, i.e., for parameter values in the range $t_+ \ll t_-$; $|a_+| \ll |a_-|$; $t_\sigma, |a_\sigma| \ll U$. This paper is an extension of the previous one.[24] In ref. 24, the chFKM (i.e., the Hamiltonian (2), (3) with $t_+ = a_+ = 0$) has been analysed. The content of ref. 24 can be summarized as follows: A perturbation theory in parameters $\frac{t_-}{U}$, $\frac{a_-}{U}$ has been applied to the chFKM, and—as a result—the *effective Hamiltonian*, up to terms proportional to U^{-3}, has been obtained. It turned out to be the classical Ising-like Hamiltonian, depending on two parameters $\bar{a} = \frac{a_-}{t_-}$, $h = \mu_+ - \mu_-$. In the next step, ground states of the effective Hamiltonian have been looked for. It was done by comparison of energies of all periodic configurations up to $N = 18$ sites per elementary cell (it corresponds to about 2×10^5 configurations). Most of these ground states have appeared in the ordinary FKM[9–11] but also a new one has emerged. It turned out that all minimal-energy configurations have no more than 5 sites per elementary cell; so it was natural to conjecture that all they are *true* ground states. However, in ref. 24 authors have not been able to prove it.

One of results of this paper is a proof of these (so far) nonrigorous results of ref. 24. The proof is based on a formulation of the effective Hamiltonian as an *m-potential*. Moreover, this result is generalized in two directions. Namely, the *thermal* and *quantum* stability of ground states is proved. More precisely, it means that

- it is shown that ground-states orderings are also present in non-zero (but sufficiently low) temperatures. In the other words, the low-temperature phase diagram will be only small deformation of the zero-temperature one;
- Moreover, the deformation of the phase diagram will be small if we allow presence of non-zero hopping terms with $t_+ \neq 0$, $a_+ \neq 0$ in the Hamiltonian, provided that they will be sufficiently small: $t_+ \ll t_-$, $|a_+| \ll |a_-|$.

These facts have been proved by an application of the *quantum Pirogov–Sinai theory*, developed in refs. 17–20. (It should be stressed that there exist another version of the quantum Pirogov–Sinai theory, developed independently in a series of papers[21, 22]).

The content of the paper is as follows. In Section 2, some basic facts concerning lattice version of perturbation theory in the formulation,[18, 20]

are reviewed. This scheme (valid for parameter range $t_\sigma \ll U$, $|a_\sigma| \ll U$) is applied to the Hamiltonian (2), (3) up to terms proportional to U^{-3}. In such generality, this Hamiltonian is too difficult to analyse; however, when we restrict ourselves to the case $|t_+| \ll |t_-|$, $|a_+| \ll |a_-|$, the rigorous analysis of the low-temperature properties can be performed. Such a Hamiltonian is the *classical* (Ising-like) one with small non-classical (Heisenberg-like) perturbation. In Section 3, ground states of the classical part of the effective Hamiltonian have been obtained. It was done by reformulating the Hamiltonian as a sum of m-potentials[10, 18, 26] constructed by adding the suitable *zero-potentials* to the initial Hamiltonian. In Section 4, general sketch of the proof of the stability of these ground states with respect to *thermal* and *quantum* perturbations has been presented. Section 5 contains the conclusions, discussion on the possibilities of extensions of results and comparison with some other papers. In Appendix A, some notions used in Section 3, are collected. Appendix B contains the list of misprints of the paper of ref. 20 (it is supplied because this paper refers frequently to ref. 20, and numerous misprints there were distracting for the author).

2. PERTURBATION THEORY AND EFFECTIVE HAMILTONIAN

2.1. General Remarks

We have to do with lattice systems described by the Hamiltonian of the form

$$H_\Lambda(\mu; \lambda) = H_{0,\Lambda}(\mu) + \lambda V_\Lambda, \tag{4}$$

where $\Lambda \subset \mathbb{Z}^d$, $H_{0,\Lambda}(\mu)$ is a *classical* operator (i.e., it can be written in diagonal form in the basis being tensor product of site bases; tensor product is taken over all sites belonging to Λ), dependent of parameter(s) μ; λ is perturbation parameter (it can be one- or many-dimensional) and λV_Λ is a small (in a suitable natural sense) quantum operator. It is assumed that both $H_{0,\Lambda}$ and V_Λ are *finite range* operators. In the other words, models under consideration are of type "classical Hamiltonian plus small quantum perturbation." Of course, this is only some subclass of quantum models; nevertheless, it contains many interesting ones (including Hubbard-like models in the atomic limit).

Let us assume that ground state(s) of H_0 possess certain ordering(s), which can depend of μ. Our two basic questions are: (i) What will happen if we consider the model in finite temperature? Will the ordering(s) disappear at arbitrary small temperature, or will they be preserved up to some critical temperature? (ii) What will happen under influence of the quantum perturbation λV_Λ?

Consider the influence of temperature first. It is possible to analyse rigorously the situation when H_0 has ground state of finite degeneracy (it can depend of μ). Assume that *Peierls condition* (described in more details below), and certain non-degeneracy conditions on coexistence lines are fulfilled. Then, the celebrated *Pirogov–Sinai theory*[26, 27] states that orderings of ground states will also be present in positive, sufficiently small temperatures. Moreover, zero-temperature phase diagram will undergo only small deformation when we pass to non-zero temperatures.

This theorem can be generalized to the situation when the classical system is perturbed by the small quantum operator. Then, if the above "classical" and also certain "quantum" Peierls conditions are fulfilled, it has been proved,[17] that also in this case the stability of ground states holds. (Related results have been established in refs. 21 and 23). In the other words, phase diagrams will be deformed in a small degree, if the temperature is sufficiently low and the quantum perturbation is sufficiently small.

One can say that sufficiently small thermal perturbations of finite-degeneracy classical systems don't destroy orderings of ground states. However, the situation changes dramatically when the classical system exhibits infinite degeneracy. (Such opportunity happens quite frequently. It takes place, for instance, for certain important regions of the Hamiltonian (2), corresponding to FKM and HuM in atomic limit.) In such situations, both thermal and quantum perturbations can lead to very complicated phenomena, which full treatment hasn't been worked out so far. However, some particular cases are tractable. One of such situations is that the degeneracy can be lifted by perturbation, and some group of states with *finite degeneracy* emerges. In this case, one can further analyse behaviour of these states, i.e., their behaviour in further orders of perturbation theory and under thermal perturbation. If we are interested only in the low-temperature behaviour of the system, then it turns out that one should know details of only ground state(s) and low-energy ones, so the full diagonalization of the Hamiltonian is not necessary. The second aspect of matter is necessity of writing of the Hamiltonian in the form of local interactions, because we must control the convergence of perturbation theory in thermodynamic limit, as we deal with lattice systems.

Perturbation theory adapted to these goals has been developed in refs. 18 and 20 and we present their main points below. (It should be noted that parallel results have been obtained in ref. 22. Results in refs. 18–20 and in ref. 22 are—in general features—physically equivalent, although they have been obtained by different approaches. The former method rely on perturbative diagonalization of the Hamiltonian in low-energy part first, and on the application (if possible) of the Pirogov–Sinai theory to the

resulting effective Hamiltonian as a next step. The approach presented in the latter paper can be viewed as a certain generalization of methods developed in ref. 33, which has been devised for examining low-temperature properties of systems with infinite ground-state degeneracy, using the notions of *dominant ground states* and *restricted ensembles*. This generalization can be viewed as taking into account in one step not only thermal perturbation but also the quantum one. In author's opinion, the DFF approach is easier to use, whereas the Kotecky *et al.* approach seems to be able to treat larger class of models—especially such ones where degeneracy is not lifted by the quantum perturbation alone. However, this is a matter of further development of this theory.)

Summarizing, there are two basic steps in the whole procedure. (1) Diagonalize the Hamiltonian in the low-energy part up to nth order, and write the result out as a sum of local objects. This way, the Hamiltonian is reformulated as a block-diagonal nth order effective Hamiltonian plus a small non-diagonal correction of the order $n+1$. This is done in this paper in this section below. (2) If nth order effective Hamiltonian is a classical one, then one should determine its ground states. If the "classical" and "quantum" Peierls conditions are fulfilled, then stability of these ground states follows. It is a content of the following two sections.

2.2. Perturbation Theory for aschHuM

We will consider the system defined on a finite subset Λ of the lattice $\mathbb{Z}^d$. Let us assume that on every lattice site $i \in \mathbb{Z}^d$ we have some Hilbert space $\mathscr{H}_i$; we assume that all these spaces $\mathscr{H}_i$ are isomorphic. The Hilbert space of the whole system $\mathscr{H}_\Lambda$ is a tensor product: $\mathscr{H}_\Lambda = \bigotimes_{i \in \Lambda} \mathscr{H}_i$.

Assume that we analyse systems in such a form that the Hamiltonian is the sum of one-site classical operators and the sum of two-site operators:

$$H_\Lambda = H_{0,\Lambda} + V_\Lambda \equiv \sum_{i \in \Lambda} \Phi_i + \sum_{X \subset \Lambda} Q_X \tag{5}$$

where Φ_i is a classical potential defined on site i. We assume that energies of collections of ground states and excited states of Φ_i are divided by sufficiently large energy gap (in the case of aschHuM it means that U is sufficiently large). X is a pair of n.n. sites; Q_X is a small quantum (in the norm sense) operator.

Remark. The procedure of generation of effective Hamiltonians and their analysis has been developed for much more general case, i.e., Q and Φ are finite-range operators (or even infinite-range ones, but exponentially

falling with distance). However, in such a case the formulas are much more complicated and we will not reproduce them in full generality. Interested reader can find them in ref. 18.

Now, we restrict ourselves to the system (2), (3). Let us begin our analysis from the classical part of the Hamiltonian, which is well known (Fig. 1; ref. 20). Every $\mathscr{H}_i$ is spanned by the states: $|n_{i,+}, n_{i,-}\rangle$ or, explicitly, $|0, 0\rangle$, $|1, 0\rangle$, $|0, 1\rangle$, and $|1, 1\rangle$. The corresponding energies are: 0; $-\mu_+$; $-\mu_-$; $U-\mu_+-\mu_-$. The phase diagram consist of the following four regions. In region I, defined by

$$\text{I: } \mu_+ < 0,\ \mu_- < 0 \tag{6}$$

all sites are empty. In two twin regions II_+, II_- given by conditions:

$$\text{II}_+\text{: } \mu_+ > 0,\ \mu_+ > \mu_-,\ \mu_- < U \tag{7}$$

(for II_-, one should interchange the subscripts $+$ and $-$) all sites are in the $|1, 0\rangle$ (corresp. $|0, 1\rangle$) state. In the region III, given by:

$$\text{III: } \mu_+ > U,\ \mu_- > U \tag{8}$$

all sites are doubly occupied.

We choose the states $|1, 0\rangle$ and $|0, 1\rangle$ as ground states, which means that we analyse the phase diagram in some subset of the region $\text{II}_+ \cup \text{II}_-$ (i.e., the shaded region on Fig. 1). The most interesting situation takes

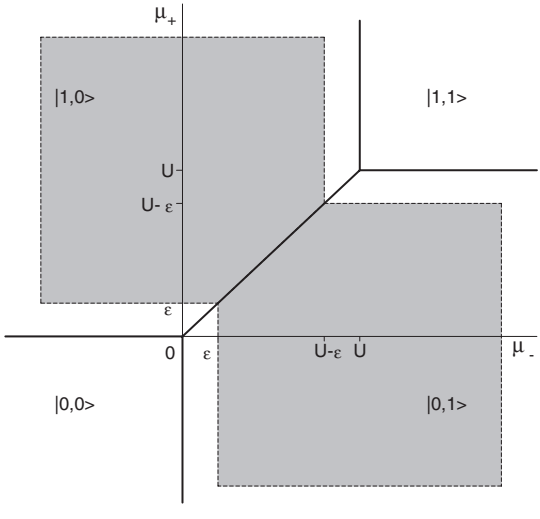

Fig. 1. Phase diagram of the nonperturbed Hamiltonian (2).

place in the neighbourhood of the $\mu_+ = \mu_-$ line between regions II_+ and II_-, where the macroscopic degeneracy is observed.

We will need the *projection operator* on ground states:

$$P_i^0 = (n_{i,+} - n_{i,-})^2. \tag{9}$$

The effective Hamiltonian has been derived up to the fourth order along the lines in ref. 20, Section 3. Their adaptation to our case turned out to be straightforward, so we reproduce here only the results.

The effective Hamiltonian is a sum of three parts.

$$H_0^{(4)} = h_0^{(0)} + h_0^{(2)} + h_0^{(4)}. \tag{10}$$

The first of them is the nonperturbed potential:

$$h_0^{(0)} = \sum_{i \in \Lambda} P_i^0 \Phi_i P_i^0. \tag{11}$$

The remaining parts contain products of creation and annihilation operators. It is convenient to express them in *spin variables*, i.e., certain bilinear combinations of creation and annihilation operators. We have:

$$\vec{\mathbf{S}}_i := \sum_{\alpha, \alpha' = +, -} c_{i,\alpha}^\dagger \vec{\boldsymbol{\sigma}}_{\alpha,\alpha'} c_{i,\alpha'} \tag{12}$$

where $\vec{\boldsymbol{\sigma}} \equiv \frac{1}{2}(\sigma_1, \sigma_2, \sigma_3)$ and $\sigma_1, \sigma_2, \sigma_3$ are standard Pauli matrices. It is convenient to use

$$S_i^3 = \tfrac{1}{2}(n_{i,+} - n_{i,-}) \tag{13}$$

and

$$S_i^\pm = S_i^1 \pm i S_i^2 = c_{i,\pm}^\dagger c_{i,\mp}. \tag{14}$$

The results below have been obtained by rather straightforward but lengthy and technical calculations with the aid of programs to symbolic computations. I am very indebted for R. Lemański for permission to use his programme for these purposes. In formulas below we denote:

$$\tilde{t}_+ := t_+ + a_+, \qquad \tilde{t}_- := t_- + a_-. \tag{15}$$

The second term in (10) is a sum of two-body interactions:

$$h_0^{(2)} = \sum_{\langle i,j \rangle \subset \Lambda} h_{0;ij}^{(2)}, \tag{16}$$

where

$$h^{(2)}_{0;ij} = \frac{\tilde{t}_+^2 + \tilde{t}_-^2}{2U}(4S_i^3 S_j^3 - P_i^0 P_j^0) + \frac{\tilde{t}_+ \tilde{t}_-}{U}(S_i^1 S_j^1 + S_i^2 S_j^2). \tag{17}$$

This expression is a Hamiltonian of the anisotropic Heisenberg model. It has a structure identical as for asHuM (see ref. 20). The correlated hopping manifests itself here only by the change ("renormalisation") of coupling constants. However, in the next nonvanishing order, qualitatively new terms emerge.

The third term in (10) is the most complicated one. It is more than one page long; it can be viewed as anisotropic generalized Heisenberg model (with two-, three-, and four-body interactions). In its general form, it is too difficult to analyse (at least for the author): still little is known rigorously for its simpler version, i.e., the ordinary Heisenberg model.

But it is possible to obtain a rigorous information on ground states *in the FK-like regime*, i.e., for $|a_+| \ll |a_-|$, $t_+ \ll t_-$. It will be subject of the following two sections. The only information we must know about the general form, is a smallness of certain matrix elements of this operator. For this reason, the formula will be not reproduced here (interested reader can obtain it from the author upon request).

3. GROUND STATES OF EFFECTIVE HAMILTONIAN

3.1. FK-Like Limit of Effective Hamiltonian

In this section ground states of strongly anisotropic limit of the effective Hamiltonian (10) is performed. One can consider it as a weak (quantum) perturbation of the purely classical chFKM. It is necessary to determine ground states and their phase diagram of the chFKM first. It has been (nonrigorously) done in ref. 24 and now proofs will be supplied.

First, let us remind the Hamiltonian for chFKM in fourth order of perturbation theory. Our analysis covers the half-filled case, i.e., $\sum_i (n_{i,+} + n_{i,-}) = |\Lambda|$. If we take the following assumptions in the expression (10): (i) we consider the half-filled case, i.e., projections can be skipped; (ii) dimension of the lattice is equal to 2; (iii) $t_+ = a_+ = 0$, then we obtain the following effective Hamiltonian for the chFKM:[24]

$$H^{(4)}_{\Lambda,\mathrm{eff}} = \tilde{h}\sum_i s_i + J_2 \sum_{d(i,j)=1} s_i s_j + J_2' \sum_{d(i,j)=\sqrt{2}} s_i s_j + J_2'' \sum_{d(i,j)=2} s_i s_j$$
$$+ J_{3,s} \sum_{\mathscr{S}_{3,ijk}} s_i s_j s_k + J_{3,b} \sum_{\mathscr{B}_{3,ijk}} s_i s_j s_k + J_4 \sum_{\mathscr{P}_{4,ijkl}} s_i s_j s_k s_l + J_0 \sum_{\mathscr{P}_{4,ijkl}} \mathbf{1} \tag{18}$$

where $h = \mu_+ - \mu_-$; $\tilde{h} = (h - 20U\alpha\tau^3)$; $\tau = \tilde{t}_-/U$; $\alpha = a_-/U$; $J_2 = U(2\tau^2 - 18\tau^4)$; $J_2' = U(6\tau^4 + 8\alpha^2\tau^2)$; $J_2'' = U(4\tau^4 + 2\alpha^2\tau^2)$; $J_{3,s} = 8U\alpha\tau^3$; $J_{3,b} = 16U\alpha\tau^3$; $J_4 = 40U\tau^4$; $J_0 = U(3\tau^4 - 10\alpha^2\tau^2)$; $\mathscr{B}_{3,ijk}$, "bent" triples of spins i, j, k (i.e., the angle between bonds ij and jk is $\pi/2$); $\mathscr{S}_{3,ijk}$, "straight" triples; $\mathscr{P}_{4,ijkl}$ is a 2×2 square plaquette on the lattice. This Hamiltonian is an Ising-like Hamiltonian with competing antiferromagnetic interactions, and the structure of ground states can be very complicated; this situation happens for instance in the case of the ANNNI model.[25] In our case, fortunately, the structure of ground states turned out to be rich but amenable to rigorous analysis.

3.2. Determination of Ground States

Ground states of the Hamiltonian (18) will be determined by suitable modification of methods borrowed from papers.[10, 11] They rely on rewriting of the Hamiltonian as a sum of *m-potentials* (for definition, see refs. 10, 11, and 26; it is reminded in the Appendix). If a given potential is an m-potential, then we are in very lucky situation, as the *local* minimality of energy (i.e., minimality on a plaquette) implies the *global* minimality on the whole lattice.

Let us rewrite the Hamiltonian (18) as a sum of potentials over (square) plaquettes 3×3:

$$H^{(4)}_{\Lambda,\,\mathrm{eff}} = \sum_{\pi \subset \Lambda} H_\pi, \tag{19}$$

where π is a 3×3 plaquette and

$$H_\pi = \frac{\tilde{h}}{9} \sum_i s_i + \frac{J_2}{6} \sum_{d(i,j)=1} s_i s_j + \frac{J_2'}{4} \sum_{d(i,j)=\sqrt{2}} s_i s_j + \frac{J_2''}{3} \sum_{d(i,j)=2} s_i s_j + \frac{J_{3,s}}{3} \sum_{\mathscr{S}_{3,ijk}} s_i s_j s_k + \frac{J_{3,b}}{4} \sum_{\mathscr{B}_{3,ijk}} s_i s_j s_k + \frac{J_4}{4} \sum_{\mathscr{P}_{4,ijkl}} s_i s_j s_k s_l + \frac{J_0}{4} \sum_{\mathscr{P}_{4,ijkl}} \mathbf{1}. \tag{20}$$

In expression above the summation is performed over all objects (single sites, pairs, triples, plaquettes) *belonging to the plaquette* π.

It turns out that the effective Hamiltonian for chFKM neither in the form (18) nor in (19), (20) is an m-potential (except situations where we have empty or full configurations, i.e., large $\tilde{h}$ fields). In order to overcome this difficulty, Kennedy[10] has proposed to pass from original Hamiltonian to the new equivalent one, which *is* an m-potential. The trick relies on addition of suitably chosen *zero-potential* to the original Hamiltonian; zero-potential is such a potential which is non-trivial and has zero-energy

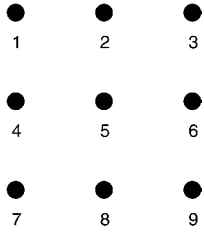

Fig. 2. Enumeration of spins on the 3×3 plaquette.

independently of configuration. Let us stress that this is a *global* condition, i.e., such that the total energy of the *whole* lattice Λ is zero (assuming periodic boundary condition); but *locally*, i.e., on the given plaquette, the energy—as a rule—is different from zero.

We will look for zero-potentials in a form analogous as in refs. 10 and 11. Let us order spin on a 3×3 plaquette as in Fig. 2.

Let us introduce the following potentials defined on these plaquettes:

$$k_1 = -s_2 - s_4 - s_6 - s_8 + 4s_5, \tag{21}$$

$$k_2 = -s_1 - s_3 - s_7 - s_9 + 4s_5, \tag{22}$$

$$k_3 = -s_1 s_3 + 2s_4 s_6 - s_7 s_9 - s_1 s_7 + 2s_2 s_8 - s_3 s_9, \tag{23}$$

$$k_4 = -s_2 s_4 - s_2 s_6 - s_4 s_8 - s_6 s_8 + s_1 s_5 + s_3 s_5 + s_5 s_7 + s_5 s_9. \tag{24}$$

It is easy to check that $k_1, \ldots, k_4$ are zero-potentials. This implies that also Ψ^0 below is a zero-potential:

$$\Psi^0 = U\left(\tilde{h} \sum_{i=1}^{4} A_i k_i + \tau^2 \sum_{i=1}^{4} B_i k_i + \tau^4 \sum_{i=1}^{4} C_i k_i + \alpha\tau^3 \sum_{i=1}^{4} D_i k_i + \alpha^2\tau^2 \sum_{i=1}^{4} F_i k_i\right) \tag{25}$$

for arbitrary collection $A_i, \ldots, F_i$. We will use this freedom to find such values of these constants that $H_\pi + \Psi^0$ is an m-potential.

Let us remind the phase diagram from ref. 24 (Figs. 3 and 4), whose validity we will prove now. We will assume the following range of the a parameter: $-1 \leqslant \bar{a} \leqslant 1$, where $\bar{a} := a_-/t_-$. This is not a principal limitation and results can be obtained also outside this region, but we limited ourselves to this parameter set, because the experimental values of $|\bar{a}|$ are less than 1—usually $|\bar{a}|$ is of the order 0.1–0.3 (see refs. 1 and 14).

There are nine phases present on the phase diagram. Five of them (0, I, II, III, and "cb") are the same as for the ordinary FK model and have their counterparts (0′, I′, II′, III′; cb is the same as cb′) obtained by interchange the full and empty sites. Moreover there exist also the new

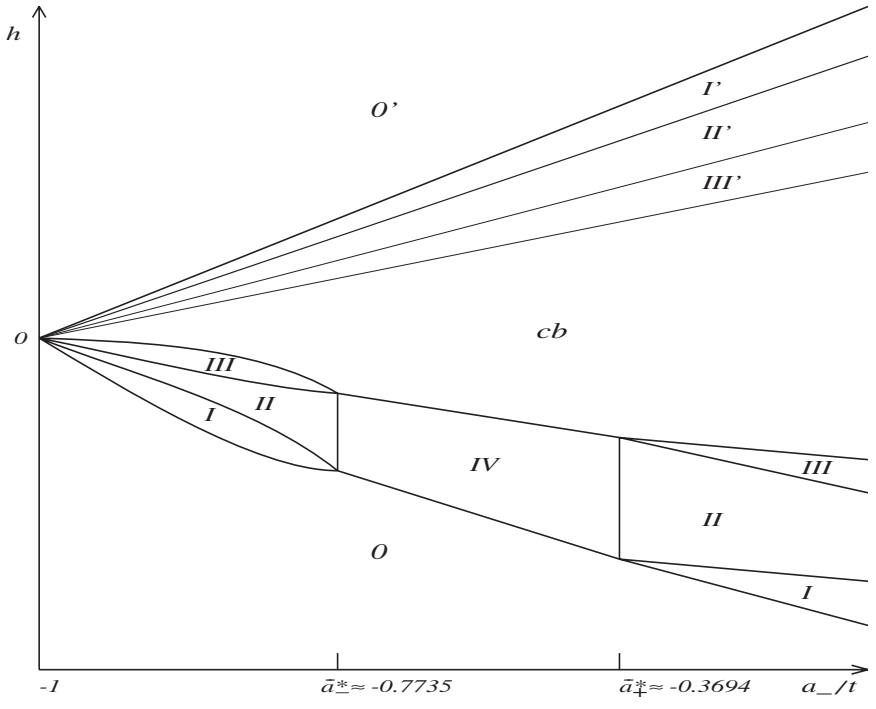

Fig. 3. Phase diagram of the fourth-order Hamiltonian (18). The phase diagram is deformed, i.e., only its topological structure is presented. The region where the "cb" phase appears possess the height of the order $\tilde{t}_{-}^{2}/U$, whereas other phases occupy regions with height of the order $\tilde{t}_{-}^{4}/U^{3}$. The h parameter is a difference of chemical potentials $\mu_{+}-\mu_{-}$.

phase denoted as IV, whereas IV′ does not appear. Orderings are shown on Fig. 4. Energies of these phases are given by the formulas:

$$E_0 = h + U(4\tau^2 + 24\tau^4 + 60\alpha\tau^3 + 20\alpha^2\tau^2) \tag{26}$$

$$E_{\mathrm{I}} = \tfrac{3}{5}h + U(\tfrac{4}{5}\tau^2 - \tfrac{136}{5}\tau^4 - 28\alpha\tau^3 + 4\alpha^2\tau^2) \tag{27}$$

$$E_{\mathrm{II}} = \tfrac{1}{2}h + U(0\tau^2 - 36\tau^4 - 42\alpha\tau^3 + 2\alpha^2\tau^2) \tag{28}$$

$$E_{\mathrm{III}} = \tfrac{1}{3}h + U(-\tfrac{4}{3}\tau^2 + 0\tau^4 - 44\alpha\tau^3 + 4\alpha^2\tau^2) \tag{29}$$

$$E_{\mathrm{cb}} = 0h + U(-4\tau^2 + 96\tau^4 + 0\alpha\tau^3 + 20\alpha^2\tau^2). \tag{30}$$

The energies for primed phases are obtained by the sign change in coefficients at h and $\alpha\tau^3$. We have also

$$E_{\mathrm{IV}} = \tfrac{1}{2}h + U(0\tau^2 - 32\tau^4 - 34\alpha\tau^3 + 4\alpha^2\tau^2). \tag{31}$$

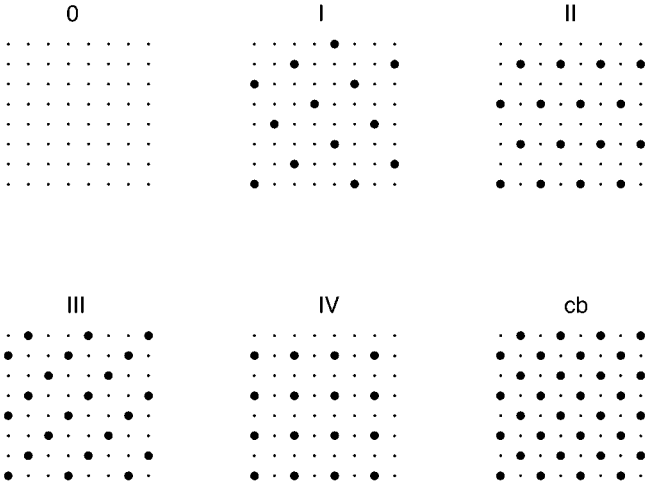

Fig. 4. Orderings appearing in the fourth-order Hamiltonian.

We will denote the line dividing ith and jth phases as $h_{i/j}$. Equations for these lines are obtained from the condition of equality of energies of ith and jth phases. Explicit expressions for $h_{i/j}$ are as follows:

$$h_{0/\mathrm{I}} = U(-8\tau^2 - 128\tau^4 - 220\alpha\tau^3 - 40\alpha^2\tau^2) \tag{32}$$

$$h_{\mathrm{I/II}} = U(-8\tau^2 - 88\tau^4 - 140\alpha\tau^3 - 20\alpha^2\tau^2) \tag{33}$$

$$h_{\mathrm{II/III}} = U(-8\tau^2 + 216\tau^4 - 12\alpha\tau^3 + 12\alpha^2\tau^2) \tag{34}$$

$$h_{\mathrm{III/cb}} = U(-8\tau^2 + 288\tau^4 + 132\alpha\tau^3 + 48\alpha^2\tau^2). \tag{35}$$

Equations for lines $h_{i'/j'}$ are obtained from those defining lines $h_{i/j}$ by reversing signs at all terms except those proportional to $\alpha\tau^3$. Moreover

$$h_{0/\mathrm{IV}} = U(-8\tau^2 - 112\tau^4 - 188\alpha\tau^3 - 32\alpha^2\tau^2) \tag{36}$$

$$h_{\mathrm{IV/cb}} = U(-8\tau^2 + 256\tau^4 + 68\alpha\tau^3 + 32\alpha^2\tau^2). \tag{37}$$

These equations have no primed counterparts, as the phase IV′ does not appear. Notice that lines: $h_{0'/\mathrm{I}'}$, $h_{\mathrm{I}'/\mathrm{II}'}$, $h_{\mathrm{II}'/\mathrm{III}'}$, $h_{\mathrm{III}'/\mathrm{cb}}$ appear for all values of $\bar{a}$, but the lines $h_{0/\mathrm{IV}}$ and $h_{\mathrm{IV/cb}}$ appear only if the condition

$$\bar{a} \in [\bar{a}_-^*, \bar{a}_+^*] \tag{38}$$

is fulfilled. Similarly, $h_{0/I}$, $h_{I/II}$, $h_{II/III}$, $h_{III/cb}$ appear values of $\bar{a}$ fulfilling

$$-1 \leqslant \bar{a} \leqslant \bar{a}_{-}^{*}, \qquad \bar{a}_{+}^{*} \leqslant \bar{a} \leqslant 1 \tag{39}$$

(two branches). In formulas above

$$\bar{a}_{-}^{*} = -\frac{4+\sqrt{2}}{7} \approx -0.773459; \qquad \bar{a}_{+}^{*} = -\frac{4-\sqrt{2}}{7} \approx -0.369398.$$

For these values of $\bar{a}$, energies of corresponding phases on the phase diagram (two coexisting phases on lines, or four coexisting phases on points) are equal.

It is clear that every lattice configuration can be built from plaquette configurations, presented on Fig. 5, and twin configurations resulting from the change of spins "+" onto "−" and vice versa (configuration 16′ or 19′ will not appear, because 16 is a twin of 19). Only configurations *without* two ions as nearest neighbours are considered due to antiferromagneticity of interactions in the second-order perturbation theory.

To proceed further, we must calculate energies of all possible plaquettes, i.e., values of functions (20), (25) on all plaquette configurations. Notice that we need *all* plaquettes, i.e., both those presented on Fig. 5 and their twins. It is so because the Hamiltonian is not invariant with respect to the change $h \to -h$. Such a computation is straightforward, but the results are lengthy and will be not reproduced here. After that, one tries to choose coefficients A_i, B_i, C_i, D_i, F_i $(i = 1,\ldots, 4)$ in such a manner that the sum $H_\pi + \Psi^0$ is an m-potential. Author couldn't find a single expression for Ψ^0 in a whole phase diagram. But it was possible to find Ψ^0 in all regions of

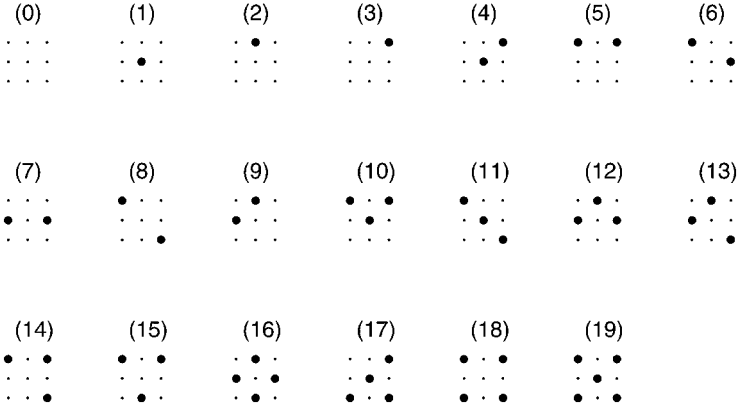

Fig. 5. Plaquette configurations.

phase diagram occupied by a single phase. This way, the covering of the whole phase diagram has been achieved.

3.3. Main Result

In this section, results concerning ground states of the effective Hamiltonian (20) in certain regions of phase diagram are formulated and proved.

Let us divide the parameter space of the phase diagram into regions: R_i ($i = 0$, I, II, III; 0′, I′, II′, III′; IV, cb) occupied by corresponding phases, according to Fig. 3. Moreover, we need to divide R_0 as: $R_0 = R_{0,1} \cup R_{0,2}$, where $R_{0,1}$ is defined by the condition: $h < h_{0/\mathrm{I}}$ and Eq. (39), whereas $R_{0,2}$ by: $h < h_{0/\mathrm{IV}}$ and Eq. (38). Similarly, $R_{\mathrm{cb}} = R^{-}_{\mathrm{cb},1} \cup R^{-}_{\mathrm{cb},2} \cup R^{+}_{\mathrm{cb}}$, where $R^{-}_{\mathrm{cb},1}$ is defined by the condition: $h_{\mathrm{III/cb}} < h \leqslant 0$ and Eq. (39); $R^{-}_{\mathrm{cb},2}$—by: $h_{\mathrm{IV/cb}} < h \leqslant 0$ and Eq. (38); R^{+}_{cb}—by: $0 \leqslant h < h_{\mathrm{IV/cb}}$.

Theorem 1. For every subregion R_i of the phase diagram, and for values of coefficients for every R_i, given in Table I, the potential: $\tilde{H}^i_\pi = H_\pi + \Psi^{0;i}$ is an m-potential. Plaquette configurations of minimal energy in every region R_i (open sets and lines) are listed in Table II. It leads to lattice configurations for every R_i as in Fig. 4.

The set of plaquettes which minimize energy on a subset S of phase diagram will be denoted by $\mathscr{E}^{\min}(S)$.

The strategy of proof is as follows:

1. First we analyse situation on boundaries $h_{i/j}$ dividing regions occupied by particular phases. Inserting values of A_i, B_i, C_i, D_i, F_i from Table I into an expression for Ψ^0, one obtains plaquette configurations minimizing energy. This way, the set $\mathscr{E}^{\min}(S)$ is determined in the case when S is a line.

2. Having $\mathscr{E}^{\min}(S)$ on boundaries $h_{i/j}$ and $h_{j/k}$, one determines those plaquette configurations which minimize energy inside the region R_j. This last fact can be checked by looking at coefficient at h; from minimality of energy on boundaries of R_j, the minimality of energies inside the region follows immediately.

3. After we have determined the set of *plaquette* configurations with minimal energy, we are looking for *lattice* configurations, which can be build from allowed plaquettes.

The following fact is helpful when one determines $\mathscr{E}^{\min}(S)$ in the case when S is a line $h_{i/j}$. Namely, it turns out that on lines: $h_{0/\mathrm{I}}$, $h_{\mathrm{I/II}}$, $h_{\mathrm{II/III}}$,

Table I. Values of Coefficients in Eq. (25) for Which the Potential: $\tilde{H}^i_\pi = H_\pi + \Psi^{0;\,i}$ Is an m-Potential in Every Region R_i

Region	A_1	A_2	A_3	A_4	B_1	B_2	B_3	B_4	C_1	C_2	C_3	C_4	D_1	D_2	D_3	D_4	F_1	F_2	F_3	F_4
$R_{0,1}$; R_{I}	$\frac{1}{5}$	$\frac{1}{5}$	$\frac{3}{20}$	0	$\frac{18}{5}$	$-\frac{12}{5}$	$\frac{6}{5}$	0	$\frac{108}{5}$	$-\frac{297}{5}$	$\frac{36}{5}$	0	44	-76	9	0	0	0	0	0
R'_0; R'_{I}	$\frac{1}{5}$	$\frac{1}{5}$	$-\frac{3}{20}$	0	$-\frac{18}{5}$	$\frac{12}{5}$	$\frac{6}{5}$	0	$-\frac{108}{5}$	$\frac{297}{5}$	$\frac{36}{5}$	0	44	-76	-9	0	0	0	0	0
R_{II}	$-\frac{1}{4}$	$\frac{7}{8}$	0	0	0	3	0	0	-18	0	-12	0	-19	$\frac{37}{2}$	-24	0	-9	$\frac{27}{2}$	-6	0
R'_{II}	$-\frac{1}{4}$	$\frac{7}{8}$	0	0	0	3	0	0	-18	0	-12	0	-19	$\frac{37}{2}$	-24	0	-9	$\frac{27}{2}$	-6	0
$R_{0,2}$; R_{IV}; $R^-_{\mathrm{cb},2}$	$-\frac{1}{4}$	$\frac{7}{8}$	0	0	0	3	0	0	0	-27	0	0	17	$-\frac{71}{2}$	0	0	0	0	0	0
R_{III}; $R^-_{\mathrm{cb},1}$	$-\frac{1}{4}$	$\frac{9}{8}$	$\frac{3}{8}$	$\frac{1}{8}$	0	5	3	1	0	-63	-84	-36	17	$\frac{7}{2}$	$-\frac{3}{2}$	$-\frac{33}{2}$	0	6	-6	-6
R'_{III}; R^+_{cb}	$-\frac{1}{4}$	$\frac{9}{8}$	$-\frac{3}{8}$	$-\frac{1}{8}$	0	-5	3	1	0	63	-84	-36	17	$\frac{7}{2}$	$\frac{3}{2}$	$\frac{33}{2}$	0	-6	-6	-6

Table II. The Set of Minimal Energy Plaquettes and Corresponding Lattice Configurations in Every Region of Phase Diagram. The Characterization of the Line $l^{\pm}_{\mathrm{III/IV}}$ Is: $a = a^*_{\pm}$, $h_{0/\mathrm{I}}(a^*_{\pm}) < h < h_{\mathrm{III/cb}}(a^*_{\pm})$

Region S	The set of plaquettes of minimal energy, $\mathscr{E}^{\min}(S)$	Configurations which can be build from minimal-energy plaquettes
$h_{0/\mathrm{I}}$	{0, 1, 2, 3, 6, 7, 8}	∞ degeneracy
R_0	{0}	0
$h_{\mathrm{I/II}}$	{1, 6, 7, 8, 15}	∞ degeneracy
R_{I}	{1, 6, 7, 8}	I
$h_{\mathrm{II/III}}$	{1, 4, 7, 11, 13, 15}	∞ degeneracy
R_{II}	{1, 7, 15}	II
$h_{\mathrm{III/cb}}$	{1, 4, 10, 11, 12, 13, 16, 17, 19}	∞ degeneracy
R_{III}	{1, 4, 11, 13}	III
R_{cb}	{16, 19}	cb
$h_{0/\mathrm{IV}}$	{0, 1, 7, 18}	0, IV
$h_{\mathrm{IV/cb}}$	{1, 7, 16, 18, 19}	IV, cb
R_{IV}	{1, 7, 18}	IV
$l^{\pm}_{\mathrm{III/IV}}$	{1, 6, 7, 15, 18}	∞ degeneracy

$h_{\mathrm{III/cb}}$, an energy of every ith (non-primed) plaquette configuration has the form: $E(i) = E_0 + c_1(i)\, B(\alpha, \tau) + c_2(i)\, \tau^4$, where $c_1(i), c_2(i)$ are either 0 or positive numbers and

$$B(\alpha, \tau) = 2\tau^4 + 4\alpha\tau^3 + \alpha^2\tau^2 \tag{40}$$

(all energies are calculated for the Hamiltonian $\tilde{H}$). It is easy to see that $B(\alpha, \tau)$ is greater than zero exactly for the condition (39), which implies that minimal energy plaquettes are those for which $c_1(i) = c_2(i) = 0$.

The situation is not so evident for lines: $h_{0/\mathrm{IV}}$, $h_{\mathrm{IV/cb}}$. But still it is simple: the energy of every plaquette is in one of the following two forms: either $E(i) = E_0 + d_1(i)\, B(\alpha, \tau)$ with d_i being 0 or negative number, or $E(i) = E_0 + \tau^2 N(\alpha, \tau)$, where $N(\alpha, \tau)$ is positively defined quadratic form in α, τ. Then, minimal energy plaquettes correspond to the first possibility with $d_1(i) = 0$.

One can also ask the following question: Expressions for Ψ^0_i are determined for regions R_i. Then, on the line $h_{i/j}$ one can take the potential either from R_i or from R_j. Which potential one should take? It turns out that the set of minimal-energy plaquettes $\mathscr{E}^{\min}(h_{i/j})$ *does not depend* of the choice of potential. This fact holds for all boundary lines.

In Table II, we list result of this procedure (i.e., sets $\mathscr{E}^{\min}(S)$) in every region of phase diagram.

For primed configurations, the reasoning is identical with one exception. Namely, energies of primed configurations are of the form: $E'(i) = E'_0 + c'_1(i)\, B'(\alpha, \tau) + c'_2(i)\, \tau^4$, where

$$B'(\alpha, \tau) = 2\tau^4 - 4\alpha\tau^3 + \alpha^2\tau^2. \tag{41}$$

One can check that $B'(\alpha, \tau)$ is greater than zero for all $\alpha \in [-1, 1]$, which implies that for $\tilde{h} > 0$ all ground states are FK-like[10] and there is no new phase IV′.

This way, we have completed determination of phase diagram for ground states for the Hamiltonian (18).

One can ask the question about a relation of the diagram above and low-temperature phase diagram of the strongly aschHuM. The answer is that these diagrams are in certain sense *very similar*. More precise description and statements will be given in the next section.

4. STABILITY OF GROUND STATES OF THE ASCHHUM

4.1. Quantum Pirogov–Sinai Method

Let us resume what has been achieved so far. We started from the Hamiltonian of the form

$$H_\Lambda(\lambda) = H_{0;\Lambda} + \lambda V_\Lambda, \tag{42}$$

where $H_{0;\Lambda}$, V_Λ are as in (2), (3), respectively. (We skip the Λ index below.) After certain unitary transformation, we have obtained the effective Hamiltonian for strongly aschHuM. It turned out to be of the form:

$$H(\lambda) = H_0^{(n)}(\lambda) + Q^{(n)}(\lambda), \tag{43}$$

where $H_0^{(n)}(\lambda)$ is the classical Hamiltonian (effective Hamiltonian for chFKM up to terms proportional to $U^{-(n-1)}$; we consider here $n = 2$ and $n = 4$) and $Q^{(n)}(\lambda)$ are small quantum corrections coming from both ion hopping terms and from higher order terms (of the order $\lambda^{(n+1)}$) in perturbation theory for the chFKM. Moreover, it turns out that the classical Peierls condition for the Hamiltonian (18) (or, more precisely, for equivalent interaction) holds.

Then, one can follow the strategy described in refs. 18 and 20 and sketched in Section 2.1: The Hamiltonian $H_0^{(n)}(\lambda)$ is treated as a classical Hamiltonian with ground states of finite degeneracy, and $Q^{(n)}(\lambda)$ is its quantum perturbation. Then, one can apply the results from ref. 17 to $H_0^{(n)}(\lambda)$, thus establishing stability of its ground states with respect to

thermal and quantum perturbations. It has been done in refs. 18 and 20. This procedure can be applied in arbitrary order of perturbation theory (we consider here orders 2 and 4).

All this machinery can be applied provided certain conditions imposed on $H_0^{(n)}(\lambda)$ and the quantum part $Q^{(n)}(\lambda)$ are fulfilled (this last group of conditions can be translated back to—easier to verify—conditions for quantum part of the starting Hamiltonian). These conditions are as follows: (i) The *Peierls condition* for classical model. Roughly speaking, it tells that *the energy of an excitation is proportional to its area*; for the formal definition, see refs. 17, 18, and 26. (ii) *Two-level Peierls condition*, described in Section 5.3 of ref. 18. (iii) Some "smallness" conditions imposed on quantum part,[20] Section 5.3.

After the collection of ground states $\omega_1,\ldots,\omega_k$ of the classical effective Hamiltonian in nth order of perturbation theory $H_0^{(n)}(\lambda)$ is determined, one can find certain objects called *truncated free energies*[20] $f'_1,\ldots,f'_k$. Each f'_i is associated to the ground state ω_i. Truncated free energies (constructed from ground states using cluster expansion procedure) are very important objects: One can think on them as objects, emerging from ground states after switching the quantum perturbation on and increasing temperature. As the perturbation is small and temperature is low, there is one-to-one correspondence between ground states and truncated free energies.

4.2. Stability of the Phase Diagram of the Strongly aschHuM

4.2.1. Phase Diagram in Order 0

The Hamiltonian in the zeroth order is given by (2). Its phase diagram is common for FKM as well as HuM and it is well known (see, for instance, ref. 20). Its most important features have been reminded in Section 2.2. Its phase diagram is reproduced on Fig. 1. Each region: I, II_+, II_-, III is occupied by one phase. These regions are determined by values of chemical potentials, given by inequalities (6)–(8). Occupation of every lattice site in every such region is $|0\rangle$, $|+\rangle$, $|-\rangle$, $|\pm\rangle$, respectively.

It is obvious that *inside* of every region, we have uniqueness of the ground state and their stability, provided that the smallness conditions for temperature and quantum perturbation are fulfilled. Note however that as we approach to lines between particular regions (coexistence lines), then the Peierls constants tend to zero, which implies that region of parameters β, λ for which stability holds shrinks to zero.

4.2.2. Phase Diagram in Order 2

An effective Hamiltonian in the second order of perturbation theory has been obtained in Sections 2.2 and 3.1. Their classical part is the same as

the antiferromagnetic Ising model in a magnetic field (see the formulas (16), (17), and (18)).

Ground state of such a Hamiltonian above are (provided that $\tilde{t}_- \equiv t_- + a_- \neq 0$) depending on values of h: full configuration, empty configuration and a *checkerboard configuration* plus its translation. The two-level Peierls condition *is fulfilled* if

$$8\frac{\tilde{t}_-^2}{U} \pm h + \mathcal{O}\left(\frac{\tilde{t}_-^4}{U^3}\right) > 0 \tag{44}$$

that is, within the whole parameter space except for bands of height of order $\tilde{t}_-^4/U^3$ around the lines $h = \pm 8\tilde{t}_-^2/U$. One can check it analogously as in ref. 20, Section 5.2.

Conditions for the quantum perturbation (i.e., ionic jump) are fulfilled if

$$\frac{\tilde{t}_+}{\tilde{t}_-},\ \frac{\tilde{t}_-}{U} < \epsilon_0 \tag{45}$$

where ϵ_0 is a small number, which tends to zero when one approaches the boundary line.

On the line $h = \pm 8\tilde{t}_-^2/U$ we have infinite degeneracy of ground states. For this reason, in this order of perturbation theory we cannot establish the structure of ground states on this line and in its neighborhood. However, we *can* get certain information in the next order of perturbation theory.

4.2.3. Phase Diagram in Order 4

In fourth order of perturbation theory, the classical Hamiltonian is given by (18). Its ground states have been determined in Section 3. In order to establish their stability, the Peierls conditions should be checked. This can be done immediately. An equivalent method is to employ theorem from ref. 28: *Any finite range m-potential with a finite number of periodic ground states satisfies the Peierls condition.* Then, the classical part satisfies both Peierls conditions. This statement holds in points of phase diagram with exclusion of vicinities of coexistence lines $h_{i/j}$ (see Eqs. (32)–(37)) of width $\tilde{t}_-^6/U^5$.

The smallness condition for the quantum part as well as the stability criterion are fulfilled for β sufficiently large and $\tilde{t}_-$ satisfying

$$\frac{\tilde{t}_+}{\tilde{t}_-},\ \frac{\tilde{t}_-}{U} < \tilde{\epsilon}_0 \tag{46}$$

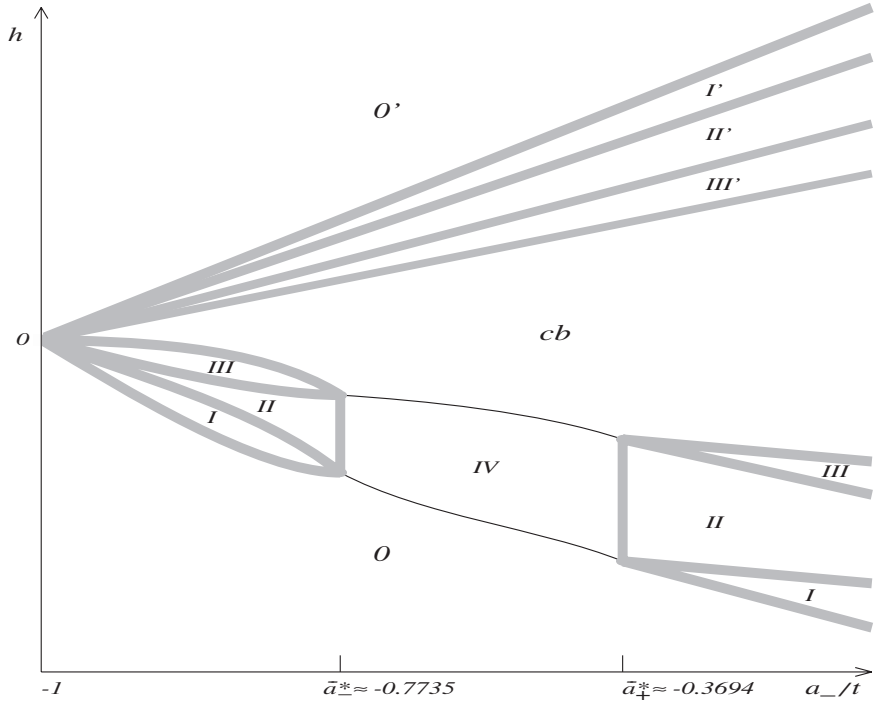

Fig. 6. Deformation of the ground-state phase diagram of the Hamiltonian (18) (see Fig. 3) under thermal and quantum perturbations. Lines: cb/*IV* and *IV*/0 will undergo only small deformation. Other phase boundaries will undergo more serious changes (splitting, appearance of new orderings), which can be investigated in next orders of perturbation theory. These regions of "terra incognita" have height of the order $\tilde{t}_-^6/U^5$ and are displayed as thick shaded lines.

(it can be checked analogously as in ref. 20, Section 5.3), i.e., the condition analogous to (45), but with smaller constant. All these arguments imply the stability of ground states (illustrated on Fig. 4) on all parameter set—except excluded stripes of height $\mathcal{O}(\tilde{t}_-^6/U^5)$ around coexistence lines of infinite degeneracy (this is illustrated on Fig. 6). This stability concerns temperature and small ion hopping.

Most of the coexistence lines on the phase diagram are lines of infinite degeneracy. But lines: 0/IV and IV/cb are exceptions: they are coexistence lines of only two configurations. It turns out that they will *not* split under perturbations and undergo only small deformation. This fact can be proved using the quantum Pirogov–Sinai theory with parameters, developed in ref. 18, Chap. 5.3. Detailed discussion, formulations and proofs can be found in ref. 18. The conditions which must be fulfilled are as follows:

(i) The Gibbs phase rule for 0-temperature phase diagram; (ii) Non-degeneracy and differentiability conditions for 0-temperature phase diagram; (iii) Estimations for smallness of derivatives of the quantum operator over parameters; (iv) the Peierls condition (with the parameter-independent constant) in the neighborhood of the coexistence line. All these conditions can be checked by straightforward calculation. As a result, we obtain that *lines* 0/IV *and* IV/cb *will undergo only small deformation under thermal or quantum perturbation.*

One can ask also further questions: It has been established that the *orderings* of ground states will be preserved under small perturbations (both thermal and quantum). What can be said about *states*? It turns out that also states of both models will share certain similarities:[20] A low-temperature equilibrium state can be visualized as a "sea" being a corresponding ground state of the classical Hamiltonian plus the fluctuatios represented by contours. Thus expectation in such a state differ little from expectation in the associated ground state of the classical Hamiltonian.

5. CONCLUSIONS AND OPEN PROBLEMS

In this paper, the structure of ground states for chFKM, established elsewhere,[24] has been proved. This result has been achieved by constructing suitable form of m-potential, similarly as in refs. 10 and 11. The second result is that these ground states are stable against increasing of the temperature and presence of quantum perturbations, such as a small ion hopping. This way, the low-temperature phase diagram of strongly asymmetric correlated-hopping Hubbard model has been obtained. These results have emerged as application of quantum Pirogov–Sinai technique, developed in refs. 17–20.

Related to the subject this work is the paper of ref. 29, where authors consider the correlated-hopping spinless 2d FK model nonperturbatively but numerically; they report results for finite systems up to 64 lattice sites. Authors claim that the segregation phenomenon have been observed (absent in our study). However, their results are obtained for relatively small values of U (up to $U = 7$) and it seems that such values of U are too small to fit the perturbative treatment presented in this paper.

It would be tempting to gain information on various generalizations of the Falicov–Kimball models, such as FK model with spin.[30] There is a significant difference between these two sorts of the model. For the spinless model, we have only two ground states (outside coexistence lines). For the model with spin, we have a macroscopic degeneracy (at least at zero external magnetic field). This is the reason that it was possible to obtain only

the effective Hamiltonian,[31] but nothing rigorous can be said about stability of these states, as the one of fundamental assumptions of the Pirogov–Sinai theory (both classical and quantum) is finite degeneracy of ground states. Notice, however, that in our case this degeneracy is in some sense "trivial," since it is lifted neither by thermal nor by quantum perturbations (provided it is independent of heavy electron spin). Quite a similar situation was reported in ref. 32, so we hope that the method used in this paper will be applicable in our situation as well. So we expect that the ground state orderings of the spin 1/2 FK model will be preserved for sufficiently low temperatures.

APPENDIX A: GROUND STATES, m-POTENTIALS

Basic notions concerning classical lattice models and quantum perturbations thereof, such as *defect set, contour, classical and quantum Peierls conditions, stability of phases* which have been used in the paper, can be found in refs. 17 and 18 (see also ref. 26). Here only definitions concerned to Section 3 are given.

Configurations. Let us consider a system defined on $\Lambda \subset \mathbb{Z}^d$, $|\Lambda| = N$. On every lattice site i we have some finite set called *classical spin* S_i. It will be assumed that all S_i are isomorphic. *A configuration* is an element of $\Omega_N = S^N \equiv \times_{i \in \Lambda} S_i$.

Classical Hamiltonian. *The Hamiltonian* H_Λ is a function defined on Ω_N. Usually Hamiltonian is defined as a sum of *potentials*, i.e., functions defined on subsets of Λ: $H_\Lambda = \sum_{B \subset \Lambda} \Phi_B$. Usually one imposes restrictions such that potentials are *finite-range* ones, i.e., such that $|B| \leqslant M$, M finite. It is also assumed that potentials are translation invariant.

m-Potential. Now, consider the system on an infinite lattice $\mathbb{Z}^d$. Assume that sets B_a (i.e., potential supports) are translation of a fixed plaquette B by a lattice vector a: $B_a = \tau_a B$, where τ_a is an operator of such translation. We say that the function Φ_B is an *m-potential*, if there exist configuration (perhaps, non-unique) $\omega^0 \in \Omega_N$ with the following properties: (i) For every plaquette B_a, the "plaquette energies," i.e., values of the Hamiltonian calculated on the plaquette B_a: $\Phi_{B_a}(\omega^0)$ are all equal; (ii) For every another configuration $\omega \in \Omega_N$, the condition: $\Phi_{B_a}(\omega^0) \leqslant \Phi_{B_a}(\omega)$ is fulfilled.

Ground States of the Classical Hamiltonian. If there exist such configuration $\omega^0 \in \Omega_N$ as above, then we call it *the ground state* of the Hamiltonian.

The property of the potential to be an m-potential can be reformulated as follows. If a given potential is an m-potential, then the *local* minimality of energy (i.e., minimality on a plaquette) implies the *global* minimality on the whole lattice. The property that a potential is an m-potential is very important one, as it replaces searching of ground states of the infinite lattice by looking for the minima on a finite set. Unfortunately, some given potential possess this property only exceptionally. A method to avoid this obstacle is to find—for a given potential Φ—an equivalent potential Φ', such that Φ' is an m-potential. However, in general it is difficult task.

APPENDIX B: MISPRINTS IN REF. 20

1. Formulas (2.72) and (2.73) should appear as:

$$V_3 = \mathrm{ad}^2 S_1 \left(\frac{V^{00}}{2} + \frac{V^R}{2} + \frac{2V^{01}}{3!} \right) \tag{2.72}$$

$$V_4 = \mathrm{ad}^3 S_1 \left(\frac{V^{00}}{3!} + \frac{V^R}{3!} + \frac{3V^{01}}{4!} \right) + \mathrm{ad}\, S_2 \left(V_2^{00} + V_2^R + \frac{V_2^{01}}{2} \right) \tag{2.73}$$

(compare ref. 18, (5.49)).

2. The formula (3.7) should appear as

$$Q_X \equiv Q_X(\underline{t}) = Q_{[xy]}(\underline{t}) + Q_{[yx]}(\underline{t}).$$

3. p. 581, an expression in the line below the formula (3.18) should be

$$V^{00}_{X_1 \cup X_2} = \tfrac{1}{2} [\mathrm{ad}\, S_{1\, B_{X_1}}(Q^{01}_{B_{X_2}}) + \mathrm{ad}\, S_{1\, B_{X_2}}(Q^{01}_{B_{X_1}})]^{00}.$$

4. p. 583, an expression in third line below the formula (3.30) should be

$$t_{\pm b} = t_{\pm \bar{b}} = t.$$

5. p. 586, Table II: In the formula for effective Hamiltonian for the Falicov–Kimball model, there should appear a term: $\frac{t^4}{2U} P^0_{\{xyzw\}}$.

ACKNOWLEDGMENTS

The author is very indebted for R. Lemański for stimulating discussions and for supplying his programme to symbolic calculations. This work was supported by the Polish State Committee for Scientific Research (KBN) under Grant No. 2P03B 13119.

REFERENCES

1. J. Hubbard, *Proc. Roy. Soc. London A* **276**:238 (1963); **277**:237 (1964); **281**:401 (1964).
2. M. C. Gutzwiller, *Phys. Rev. A* **137**:1726 (1965).
3. E. H. Lieb, *Advances in Dynamical Systems and Quantum Physics*, Proc. of the May 1993 Conference in honour of G. F. Dell'Antonio (World Scientific).
4. L. M. Falicov and J. C. Kimball, *Phys. Rev. Lett.* **22**:997 (1969).
5. C. Gruber and N. Macris, *Helv. Phys. Acta* **69**:851 (1996).
6. J. Jędrzejewski and R. Lemański, *Acta Phys. Polon. B* **32**:3243 (2001).
7. J. K. Freericks, E. H. Lieb, and D. Ueltschi, *Comm. Math. Phys.* **227**:243 (2002).
8. T. Kennedy and E. H. Lieb, *Phys. A* **138**:320 (1986).
9. Ch. Gruber, D. Ueltschi, and J. Jędrzejewski, *J. Stat. Phys.* **76**:125 (1994).
10. T. Kennedy, *Rev. Math. Phys.* **6**:901 (1994).
11. Ch. Gruber, N. Macris, A. Messager, and D. Ueltschi, *J. Stat. Phys.* **86**:57 (1997).
12. K. Haller and T. Kennedy, *J. Stat. Phys.* **102**:15 (2001).
13. J. Spałek, *Eur. J. Phys.* **21**:511 (2000).
14. J. E. Hirsch, *Physica C* **158**:236 (1989).
15. K. Michielsen, *Phys. Rev. B* **50**:4283 (1994). P. Farkasovsky, cond-mat/9908094. A. Schiller, *Phys. Rev. B* **60**:15660 (1999). K. Michielsen and H. de Raedt, *Phys. Rev. B* **59**:4565 (1999).
16. A. A. Aligia, L. Arrachea, and E. R. Gagliano, *Phys. Rev. B* **51**:13774 (1995). J. C. Amadon and J. E. Hirsch, *Phys. Rev. B* **54**:6364 (1996). L. Didukh, V. Hankevych, and Yu. Skorenkyy, *Physica B* **284–288**:1537 (2000). M. Kollar and D. Vollhardt, *Phys. Rev. B* **63**:045107 (2001).
17. N. Datta, R. Fernandez, and J. Fröhlich, *J. Stat. Phys.* **84**:455 (1996).
18. N. Datta, L. Rey-Bellet, J. Fröhlich, and R. Fernandez, *Helv. Phys. Acta* **69**:752 (1996).
19. J. Fröhlich and L. Rey-Bellet, *Helv. Phys. Acta* **69**:821 (1996).
20. N. Datta, R. Fernandez, and J. Fröhlich, *J. Stat. Phys.* **96**:545 (1999).
21. C. Borgs, R. Kotecky, and D. Ueltschi, *Comm. Math. Phys.* **181**:409 (1996). C. Borgs and R. Kotecky, *Comm. Math. Phys.* **208**:575 (2000). Ch. Gruber, R. Kotecky, and D. Ueltschi, *J. Phys. A: Math. Gen.* **33**:7857 (2000).
22. R. Kotecky and D. Ueltschi, *Comm. Math. Phys.* **206**:289 (1999).
23. A. Messager and S. Miracle-Sole, *Rev. Math. Phys.* **8**:271 (1996).
24. J. Wojtkiewicz and R. Lemański, *Phys. Rev. B* **64**:233103 (2001).
25. W. Selke, *Phase Transitions and Critical Phenomena*, Vol. 14, C. Domb and J. Lebowitz, eds. (Academic Press, London/New York, 1992).
26. J. Slawny, *Phase Transitions and Critical Phenomena*, Vol. 11, C. Domb and J. Lebowitz, eds. (Academic Press, London/New York, 1987).
27. S. A. Pirogov and Ya. G. Sinai, *Teor. Mat. Fiz.* **25**:358 (1975); **26**:61 (1976).
28. W. Holsztynski and J. Slawny, *Comm. Math. Phys.* **61**:177 (1978).
29. P. Farkašovský and N. Hudáková, cond-mat/0107105.
30. U. Brandt, A. Fledderjohann, and G. Hülsenbeck, *Z. Phys. B* **81**:409 (1990). V. Zlatić, J. K. Freericks, R. Lemański, and G. Czycholl, *Philos. Mag. B* **81**:409 (2001).
31. R. Lemański and J. Wojtkiewicz, *Phys. Stat. Sol.* **236**:408 (2003).
32. J. Jędrzejewski, *Z. Phys. B, Condens. Matter* **59**:325 (1985); *Physica A* **205**:702 (1994).
33. J. Bricmont and J. Slawny, *J. Stat. Phys.* **54**:89 (1989).