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Phase Diagram of the Two-dimensional t–t' Falicov-Kimball Model

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The ground-state phase diagram of the two-dimensional Falicov-Kimball model with nearest-neighbour and next-nearest-neighbour hoppings has been studied in the perturbative regime where hoppings are small compared with the on-site Coulomb interaction. The phase diagram at fourth-order exhibits a richer structure than the one of the ordinary Falicov-Kimball model.

KEY WORDS: Tight-binding models; Falicov-Kimball model; Perturbation expansions; Phase diagrams; Pirogov-Sinai theory.
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1. INTRODUCTION

The Falicov-Kimball model has been proposed in 1969 to description the metal-insulator transition[1]. Later on, it has been applied in another important problems: mixed valence phenomena[2], crystallization and alloy formation[3] and others. In the simplest version of this model, we are dealing with two types of particles defined on a d-dimensional simple cubic lattice $\mathbb{Z}^d$: immobile "ions" and itinerant spinless "electrons". There exist also other interpretations of the model[3,4].

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

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

where

$$H_{0,\Lambda} = U \sum_{x\in\Lambda} w_x n_x - \mu_i \sum_{x\in\Lambda} w_x - \mu_e \sum_{x\in\Lambda} n_x, \tag{2}$$

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$$V_\Lambda = -\sum_{\langle x,y\rangle\in\Lambda} t(c_x^\dagger c_y + c_y^\dagger c_x) \tag{3}$$

Here $c_x^\dagger$ and c_x are creation and annihilation operators of an electron at lattice site $x \in \Lambda$, satisfying ordinary anticommutation relations. The corresponding number particle operator is $n_x = c_x^\dagger c_x$. w_x is a classical variable taking values 0 or 1; it measures the number of ions at lattice site x. The chemical potentials of the ions and electrons are μ_i and μ_e, respectively.

The Falicov-Kimball model in its basic, "backbone" form given by (2), (3) is too oversimplified to give quantitative predictions in real experiments. However, it is nontrivial lattice model of correlated electrons and captures many aspects of behaviour of such systems. It allows rigorous analysis in many situations; for a review, see ref. 4. One can hope that a good understanding of this simpler model might lead to better insight into the Hubbard model, where rigorous results are rare [5].

One can try to make the FK model more realistic by adding various terms to the "backbone" hamiltonian (2), (3) in the manner analogous to that in the original Hubbard paper[6]. (Other possibility is enlargement of the space of internal degrees of freedom[4], but we will not consider it here.) The most important among them are: consideration of another types of lattice, particle statistics and presence of magnetic field[7]; correlated hopping (analysed in ref. 8–10); taking into account the Coulomb interactions between ions[11], as well as (small) hopping of heavy particles[12,25]; consideration of the next-nearest-neighbour hoppings (let's name this modification as the $t - t'$ model in analogy with the corresponding version of the Hubbard model[13]). This last effect has been analysed in only few papers. In ref. 14, authors established that if $t' \ll t$, then the phase diagram of the $t - t'$ FKM does not differ too much from the diagram of the pure FK model. A remarkable paper[15] is devoted to analysis of three-dimensional strongly asymmetric Hubbard model (i.e. generalized FK one) with three hopping parameters, for large Coulomb interaction constant U, in the neighbourhood of the symmetry point. Authors have determined rigorously the phase diagram in the space of parameters – hopping constants. Their analysis resembles the second order perturbation theory, but in fact goes far beyond it: authors have proven that higher orders will not modify the phase diagram obtained by the use of the Hamiltonian truncated at the second order. Moreover, they have proven that the phase diagram is also stable with respect to the small quantum and thermal perturbations.

In this paper, author examined influence of further terms of perturbation expansion (3-rd an 4-th ones) on the ground-state phase diagram in two-dimensional situation in the half-filling case, i.e. when the average value of the total particle number $\sum_{x\in\Lambda}(n_x + w_x)$ is equal to the number of sites $|\Lambda|$. Effects of higher-order-terms turned out to be very interesting in the ordinary FK model[7,16,17], where a whole collection of rigorous results, concerning properties of ground

states and low-temperature behaviour, has been obtained. At present, there exist well established techniques providing such information for certain class of quantum lattice models. They have been developed in two series of papers: by Kotecký et al.[12,21] and Datta et al.[22–25](one should mention also earlier achievements:[7,16,17]). In this paper, the methodology taken from papers[22–25] is used. It consists of three main steps:

1. Using certain version of perturbation theory, one constructs the *effective Hamiltonian*. In the case of FK models, effective Hamiltonian can be expressed in classical one-half spin variables (it is an Ising model with complicated interactions).
2. For such a Hamiltonian, one constructs zero-temperature (ground-state) phase diagram.
3. One tries to prove *Peierls conditions*. Roughly speaking, they guarantee that the ground state is divided by finite energy gap from excited ones. Moreover, they give geometric description of low-lying excited states in geometric terms (*contours*). If this step is successful, then the *quantum Pirogov-Sinai* theory guarantees the stability of ground-state phase diagram. More precisely, the $T = 0$ phase diagram of truncated Hamiltonian differs only in a small degree from the low-temperature phase diagram of the full Hamiltonian, including all orders of perturbation theory.

In this paper, the programme above has been partially realized for the $t - t'$ Falicov-Kimball model up to fourth order of perturbation theory.

As a first step of the study, the *effective Hamiltonian* has been derived; it can be written as the Hamiltonian for the Ising model with complicated interactions, leading to strong frustration. After that (step 2), ground states of the Hamiltonian have been looked for, and the phase diagram has been constructed. In the orders 2 and 3 it was possible to determine it rigorously for the whole phase diagram. In the fourth order, some regions have been determined rigorously, whereas for the remaining part, orderings have been established with the use of the *restricted phase diagram* method. The fourth-order phase diagram turned out to be more complicated than in the case of the ordinary FKM; the nnn hopping influences the phase diagram in a very strong manner. And last (step 3), Peierls conditions have been established for *some* regions of phase diagram (six phases among thirteen present on phase diagram), thus giving rigorous stability of these phases. For some other four phases, Peierls conditions have not been established, but their validity is rather convincing,as follows from restricted phase diagram method analysis. For the remaining, very small part of the phase diagram (occupied by three phases), ground states are degenerate. In order to analyse this region of the full system, it is necessary to go into further orders of perturbation theory.

The outline of the paper is as follows. In the Section 2, the effective Hamiltonians up to fourth order perturbation theory have been derived. In the Sections 3

and 4 ground states and phase diagram of the effective Hamiltonians in subsequent orders have been determined. Moreover, effects of neglected higher-order-terms as well as temperature have been discussed. The last Section 5 contains summary and conclusions, and the Appendix – some technical considerations concerning (pseudo)symmetries of the phase diagrams for effective Hamiltonians.

2. PERTURBATION THEORY AND EFFECTIVE HAMILTONIAN

2.1. Nonperturbed Hamiltonian, Their Ground States and Phase Diagram

Let us write explicit form of Hamiltonian we will work with:

$$H_\Lambda = -\sum_{d(x,y)=1} t(c_x^\dagger c_y + c_y^\dagger c_x) - \sum_{d(x,y)=\sqrt{2}} t'(c_x^\dagger c_y + c_y^\dagger c_x) + U\sum_{x\in\Lambda} w_x n_x$$
$$- \mu_i \sum_{x\in\Lambda} w_x - \mu_e \sum_{x\in\Lambda} n_x, \tag{4}$$

In this paper we examine the model in the range of parameters $t, t' \ll U$. We will assume that $t'/t \in [-1, 1]$. This is not principal limitation. However, in real systems, the value of t' is usually smaller than that of t, although both quantities are of the same order.

For derivation of the effective Hamiltonian, the method worked out in the paper[23] has been applied. It has this advantage that it can serve (provided certain conditions are fulfilled) as a first step to application of the quantum Pirogov-Sinai method and proving thermal and quantum stability of ground states. Detailed description of all these procedures can be found in ref. 22–25. Here, only the application of the method and results will be given, as the general scheme is identical as in the paper[25].

To obtain the final expression, we must divide states of the system onto *ground* and *excited* ones, and to find corresponding *projections* onto both groups. These collection of states are identical as in ref. 25.

Let us begin our analysis starting from the classical part of the Hamiltonian (2); it is well known, see ref. 25. The Hilbert space $\mathcal{H}_x$ on the x-th site is spanned by the states: $|w_x, n_x\rangle$ or, explicitely, $|0, 0\rangle$, $|1, 0\rangle$, $|0, 1\rangle$ and $|1, 1\rangle$. The corresponding energies are: $0; -\mu_i; -\mu_e; U - \mu_i - \mu_e$. The phase diagram consist of the following four regions. In region I, defined by $\mu_i < 0, \mu_e < 0$, all sites are empty. In two twin regions II_+, II_- given by conditions: II_+: $\mu_i > 0$, $\mu_i > \mu_e$, $\mu_e < U$ (for II_-, one should interchange the subscripts e and i) all sites are in the $|1, 0\rangle$ (corresp. $|0, 1\rangle$) state. In the region III, given by: $\mu_i > U$, $\mu_e > U$, all sites are doubly occupied. This situation is illustrated on Fig. 1.

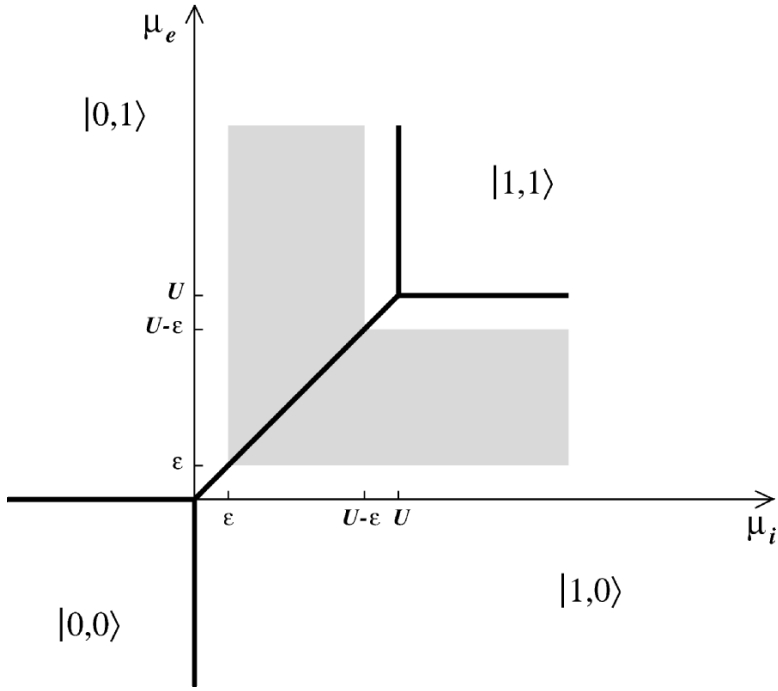

Fig. 1. Phase diagram of the nonperturbed Hamiltonian (2).

We choose the stats $|1, 0\rangle$ and $|0, 1\rangle$ as ground states. They are separated from excited ones by energy gap $\Delta = \min(\mu_i, \mu_e, U - \mu_i, U - \mu_e)$. It means that we analyse the phase diagram in some subset of the region $II_+ \cup II_-$ (the shaded region on the Fig. 1). The most interesting situation takes place in the neighbourhood of the $\mu_i = \mu_e$ line between regions II_+ and II_-; on this line, we observe a macroscopic degeneracy.

The projection operator on ground states at x-th site is

$$P_x^0 = (w_x - n_x)^2 \tag{5}$$

2.2. Effective Hamiltonians up to 4-th Order of Perturbation Theory: d = 2

Expression for effective Hamiltonian in fourth-order perturbation theory at half-filling for the ordinary FK model (in arbitrary dimension) can be found in (25), Table 2. The 4-th order effective Hamiltonian for $t - t'$ FKM can be derived using the same methodology, described in ref. 25, Sections. 2 and 3; for this reason,

details will be not repeated here. (It should be stressed that expressions up to 4-th order have been derived, for the $d = 3$ model, in the paper (15). Unfortunately, authors didn't analyse effects of orders 3 and 4).

As a final result of calculations, one obtains (from now on, the lattice dimension is equal to 2):

- Second-order correction:

$$H_0^{(2)} = -h \sum_x S_x + \sum_{d(x,y)=1} \frac{t^2}{2U} \left(4 S_x^3 S_y^3 - \mathbf{1}\right) + \sum_{d(x,y)=\sqrt{2}} \frac{t'^2}{2U} \left(4 S_x^3 S_y^3 - \mathbf{1}\right) \tag{6}$$

  where: $h = \mu_i - \mu_e$; S_x is the classical one-half spin on the lattice site x; it is related to the variable w_x by the formula: $S_x = (2w_x - 1)/2$.
- Third-order correction:

$$H_0^{(3)} = \frac{t^2 t'}{U^2} \sum_{x,y,z} \left(6\, S_x S_y S_z - \frac{1}{2}(S_x + S_y + S_z)\right) \tag{7}$$

  where summation is performed over all triples $\{x, y, z\}$ of lattice sites such that $\{x, y\}$ and $\{y, z\}$ are nearest neighbour bonds forming the angle $\pi/2$.
- Fourth-order correction is the most complicated one and is a sum of two-body (2b) and four-body (4b) interactions:

$$\begin{aligned} H_0^{(4)} = {} & C|\Lambda| + J_1^{2b} \sum_{d(x,y)=1} S_x^3 S_y^3 + J_2^{2b} \sum_{d(x,y)=\sqrt{2}} S_x^3 S_y^3 + J_3^{2b} \sum_{d(x,y)=2} S_x^3 S_y^3 \\ & + J_4^{2b} \sum_{d(x,y)=\sqrt{5}} S_x^3 S_y^3 + J_5^{2b} \sum_{d(x,y)=\sqrt{8}} S_x^3 S_y^3 + J_1^{4b} \sum_{\pi_1(xyzw)} S_x S_y S_z S_w \\ & + J_2^{4b} \sum_{\pi_2(xyzw)} S_x S_y S_z S_w + J_3^{4b} \sum_{\pi_3(xyzw)} S_x S_y S_z S_w \\ & + J_4^{4b} \sum_{\pi_4(xyzw)} S_x S_y S_z S_w \end{aligned} \tag{8}$$

In formulas above, we have: $C = 3\tau/2 + 5\tau' + 3\tau''/2$; $J_1^{2b} = -18\tau - 32\tau'$; $J_2^{2b} = 6\tau - 36\tau' - 18\tau''$; $J_3^{2b} = 4\tau - 4\tau' + 6\tau''$; $J_4^{2b} = 12\tau'$; $J_5^{2b} = 4\tau''$; $J_1^{4b} = 40\tau + 80\tau'$; $J_2^{4b} = 40\tau''$; $J_3^{4b} = 40\tau'$; $J_4^{4b} = 40\tau'$, where: $\tau = t^4/U^3$; $\tau' = t^2 t'^2/U^3$; $\tau'' = t'^4/U^3$. The four-site sets $\pi_\alpha(xyzw)$ are defined in the following way: π_1 ("square") is formed by spins occupying vertices $(0, 0)$, $(0, 1)$, $(1, 1)$ and $(1, 0)$; π_2 ("diagonal square") is formed by: $(0, 0)$, $(1, 1)$, $(0, 2)$ and $(-1, 1)$; π_3

("big triangle"): (0, 0), (0, 1), (0, 2) and (1, 1); π_4: ("rhomb") (0, 0), (1, 0), (2, 1) and (1, 1). The summation over four-body interactions in (8) is performed over all sets obtained from plaquettes $\pi_1, \ldots, \pi_4$ above by operations compatible with lattice symmetries (translations, rotations by multiple of $\pi/4$, reflections, inversions); the plaquette $\pi_\alpha(xyzw)$ occupies sites x, y, z, w.

3. GROUND STATE PHASE DIAGRAMS IN ORDER 2 AND 3

3.1. Order 2

The ground-state phase diagram of the system described by the Hamiltonian (6) can be obtained by rewriting the Hamiltonian in the following equivalent form:

$$H_0^{(2)} = \sum_{\pi_1(xyzw)} h_{0;xyzw}^{(2)} + C'|\Lambda|, \tag{9}$$

where C' is a constant and

$$\begin{aligned} h_{0;xyzw}^{(2)} = \; & \frac{t^2}{U}(S_xS_y + S_yS_z + S_zS_w + S_wS_x) + \frac{2t'^2}{U}(S_xS_z + S_yS_w) \\ & -\frac{h}{4}(S_x + S_y + S_z + S_w) \end{aligned} \tag{10}$$

(lattice sites x, y, z, w are arranged anticlockwise on the plaquette).

It is easy to check that the Hamiltonian rewritten in the form (10) is an *m-potential*[22,23,26]. If we encounter such an opportunity, we can replace the process of minimization of energy over the whole lattice by the problem much simpler: the minimization of energy over the set of plaquette configurations. These

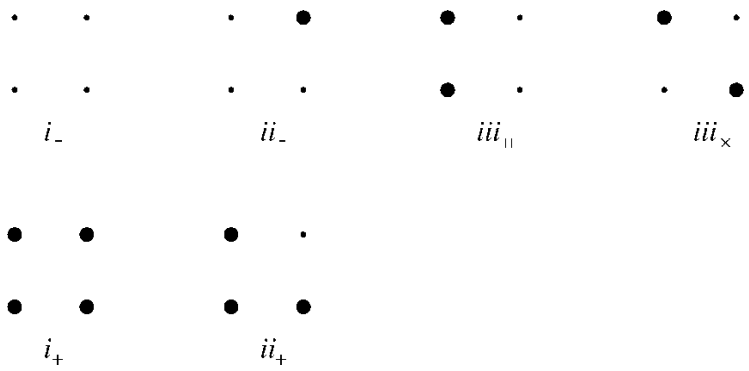

Fig. 2. Possible configurations of 2×2 plaquettes. For plaquettes *ii* and *iii* one should take into account plaquettes obtained from those illustrated above by rotations. Small dots denote empty lattice sites (or spins "down" in the spin language), big dots – occupied lattice sites (spins "up", respectively).

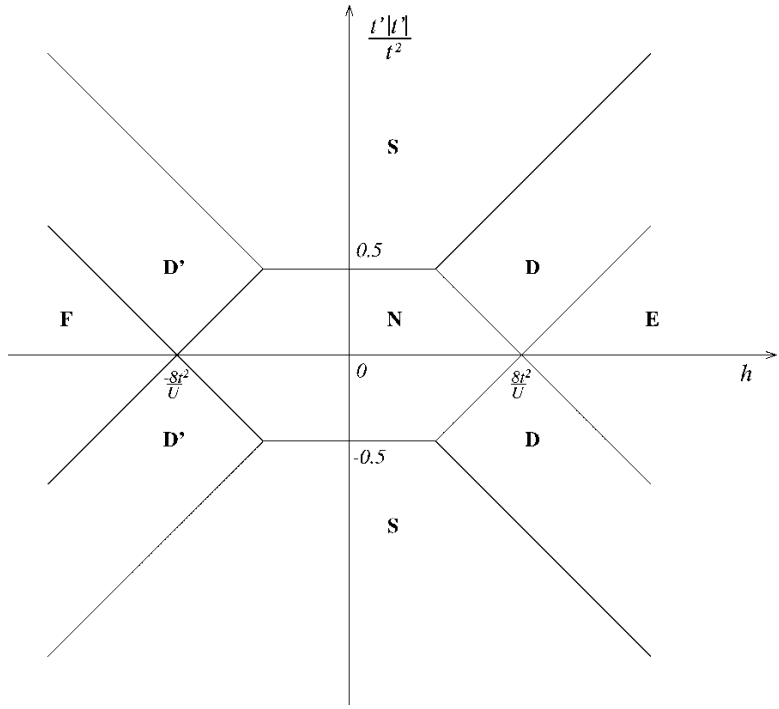

Fig. 3. Ground state phase diagram in the second order perturbation theory for the Hamiltonian (9), (10). h is the difference of chemical potentials. Phases: **E** ("empty"), **F** ("full"), **N** ("Néel") and **S** ("stripe") are unique (modulo rotations and translations), whereas phases **D**, **D**′ are macroscopically degenerate. In order 3, the phase diagram is a small deformation of the above picture.

configurations are presented on Fig. 2. It leads to the picture of the phase diagram as illustrated on Fig. 3. This diagram possess two obvious symmetries. One of them is due to symmetry of the hamiltonian (6) with respect to the change of sign $t' \to -t'$; the phase diagram is also symmetric with respect to such a change of sign. The second one is the symmetry of phase diagram with respect to the change $h \to -h$; however, in this case, one should also replace configurations by their mirror images (i.e. $S_x \to -S_x$).

Phases **E** ("Empty") and **F** ("Full") are built from plaquettes i_+ and i_-, respectively (the **E** phase is the configuration $N^o = 0$ on the Fig. 4). These phases are *unique*. We have similar situation for regions **N** ("Néel" phase; Fig. 4, configuration $N^o = 10$) and **S** ("Stripe"; see Fig. 4, configuration $N^o = 11$, which can be considered as an analogon of the "planar" phase in ref. 15). They are build from plaquettes $iii_\times$ and $iii_{||}$, respectively. Again, these phases are unique (modulo translations).

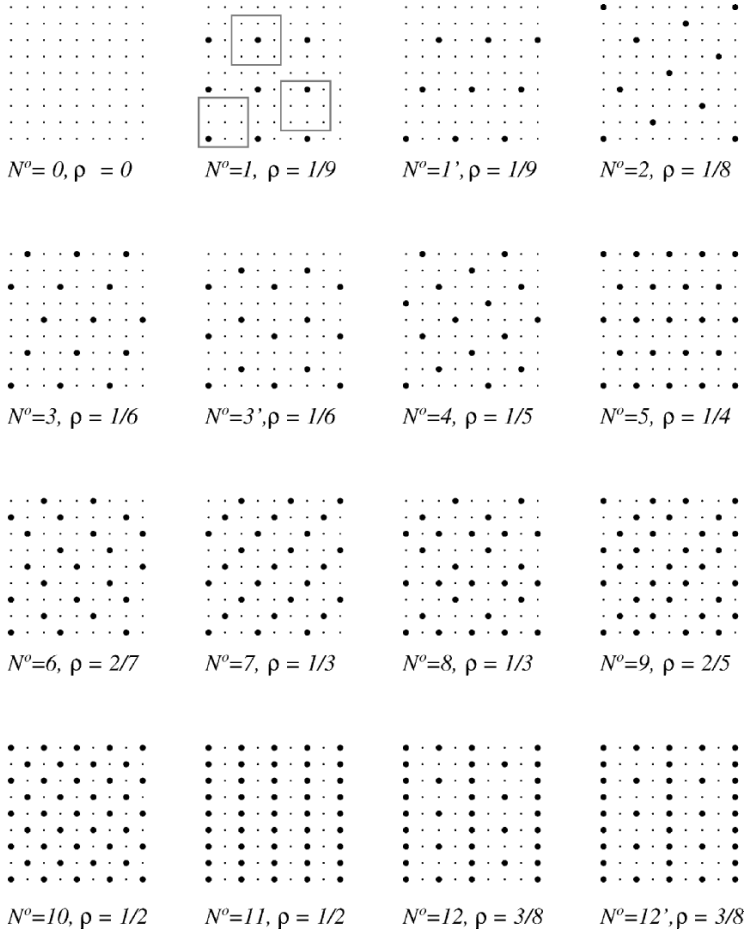

Fig. 4. Phases appearing on the ground-state phase diagram for the fourth-order effective Hamiltonian (8). Configurations: 0,2,4–11 are unique modulo lattice symmetry operations. Configurations possessing densities $1/9$, $1/6$ and $3/8$ are degenerate and form infinite series; two first examples for every such a series are shown (1,1′ etc.). Plaquette configurations being 'building blocks' for phases of density $1/9$ are drawn on the lattice configuration $N^o = 1$.

The situation for phases **D** and **D**′ is different. These phases are build from plaquettes ii_+, ii_-, respectively (see Fig. 4, configuration $N^o = 5$ as an example). However, they are *non-unique*, as there is a large dose of freedom in building of lattice configurations from these plaquettes. As a result, these phases are macroscopically degenerate. We encounter similar situation as for the antiferromagnetic Ising model on triangular lattice.

3.2. Order 3

Now, let us check how the phase diagram will change under switching third-order terms on. Let us rewrite the third-order correction (7) in the equivalent "plaquette" form:

$$H_0^{(3)} = \sum_{\pi_1(xyzw)} h_{0;xyzw}^{(3)} \tag{11}$$

where

$$\begin{aligned} h_{0;xyzw}^{(3)} = & \frac{6\,t^2t'}{U^2}(S_xS_yS_z + S_yS_zS_w + S_zS_wS_x + S_wS_xS_y) \\ & - \frac{3\,t^2t'}{2U^2}(S_x + S_y + S_z + S_w) \end{aligned} \tag{12}$$

(again spins x, y, z, w are arranged anticlockwise on the plaquette).

The full Hamiltonian, up to third-order terms, is the sum of terms (10) and (12). As in previous Subsection, one can check that it is an m-potential. Moreover, it turns out that the presence of third-order terms *does not modify ground states of plaquettes*. In the other words, plaquette configurations which were ground-states in the second order, remain ground states also in third order! This implies that degeneracy of phases **D** and **D**′ *is not lifted* and they still are degenerate. What *does* change, it is location of the boundary between phases. The difference in location of phase boundaries in orders 2 and 3 is of the order t^2t'/U^2.

The phase diagram in third order possess certain kind of symmetry. It is discussed in more details in the Appendix. At this moment, we only conclude that *the phase diagram in 3. order is a small deformation of the second-order phase diagram*.

4. PHASE DIAGRAM IN FOURTH ORDER

Regions occupied by phases **D, D**′ in both second and third order exhibit macroscopic degeneracy. One can expect that they are sensitive against perturbations and that in some of next orders this degeneracy will be lifted. It happens yet in fourth order; we describe the situation below.

This picture has been obtained by the *restricted phase diagram* method[9,18,19,20]. Recall that in this method, one takes into account all periodic configurations up to certain values of lattice sites N per elementary cell, and then one minimizes the energy over this set of configurations. For phases: 0, 4, 5, 7, 10, 11 these results have been also made rigorous by construction of m-potentials.

The ground-state phase diagram is much more complicated than for the ordinary FKM – see Figs. 4 and 5 but it is still manageable (in some respects

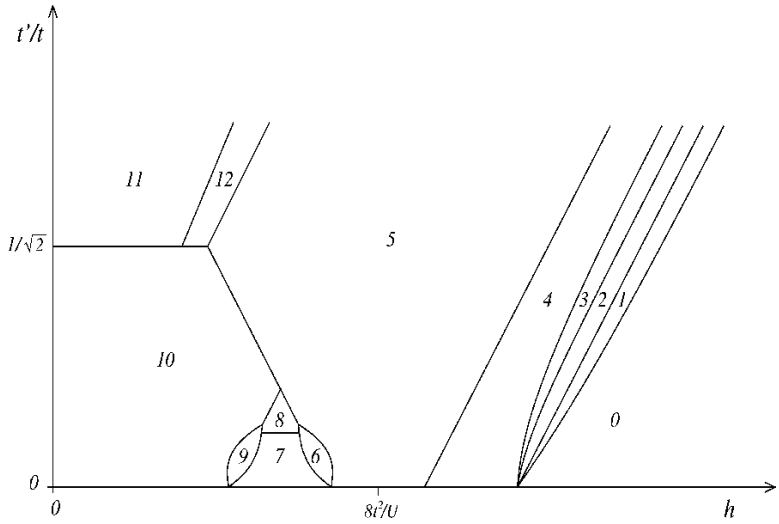

Fig. 5. The ground-state phase diagram for the fourth-order effective Hamiltonian (8). Only topological aspects of the phase diagram are displayed, as most of phases occupy very narrow regions. Phases: 1–4, 6–9 and 12: width of these regions is of fourth order in expansion parameter; other phases occupy regions of width of the second order in expansion parameter. Only one quarter (i.e. values $h > 0, t' > 0$) are shown, as for other quarters, topological structure of the phase diagram is the same.

it is similar to the phase diagram of the FKM on triangular lattice, studied in ref. 7). Thirteen phases have been detected on phase diagram; three of them are degenerate. Moreover, for each phase present for $h > 0$, there corresponds their "mirror" for $h < 0$ (this mirror is obtained by the change of occupied sites onto unoccupied ones and vice versa). For non-degenerate phases, number of sites per elementary cell does not exceed 12. Such a picture emerged at $N = 12$ (it corresponds to 2000 trial configurations) and hasn't changed up to $N = 27$ (where more than 3×10^7 trial configurations has been taken into account). This opportunity strongly suggests that the phase diagram in fourth-order is exact, i.e. that configurations present on phase diagram are true minimizers among *all* configurations.

The phase diagram in fourth order possess certain (pseudo)symmetries. Considerations concerning this aspect are somewhat lengthy and technical, so they have been relegated to the Appendix. Let us summarize the picture by the statement that the topological structure of phase diagram is the same for $h > 0$ and $h < 0$; for every phase i appearing for $h > 0$, we have corresponding mirror $\hat{i}$ for $h < 0$. Differences in location of boundary lines are of the order $p_4(t, t')/U^3$ (where $p_4(t, t')$ is some homogeneous fourth-order polynom in t and t').

A very interesting effect of the presence of the term with next-nearest-neighbour hopping is the appearance of the anomally large region occupied by the phase 5 (FK-like phase with density $1/4$). At first sight, phases appearing in the fourth-order perturbation theory should occupy region of the width $p_4(t, t')/U^3$. However, it turns out that phase 5 occupies a region of width proportional to t'^2/U, i.e. of the same order as the Néel phase, appearing in the second order! One can explain this phenomenon in the following way: Regions occupied by phase **D** (the situation for phase **D**′ is analogous) has width of the order t'^2/U both in 2-nd and in 3-rd order. The fourth-order perturbation lifts this degeneracy. As a result, the phase **D** (an 'ancestor') transforms into non-degenerate phase 5 (the 'descendant') of the same density, and occupies region approximately as large as an 'ancestor' **D**.

Most of ordered phases present on the phase diagram is unique (modulo symmetries, i.e. translations and rotations compatible with lattice structure) but also phases degenerate even in the 4-th order (phases 1, 3, 12) have been observed. More precisely, the restricted phase diagram method detects here only *finite* degeneracy, i.e. finitely many ground states with identical energy and density but different orderings (we don't count trivial degeneracy due to symmetry operations, i.e. translations, rotations and reflections). Number of these ground states grows with N; for $N = 27$ we observed: eight phases of equal energy and density $1/9$, (the first two such configurations are phases 1 and $1'$); eight phases of density $1/6$ (the first two such configurations are phases 3 and $3'$); five phases of density $3/8$ (the first two of them are 12 and $12'$).

In thermodynamic limit, number of these phases grows to infinity. It can be seen using the following arguments (the reasoning below is in fact due to one of anonymous referees; I am very indebted for this remark). First, remember that the range of interactions in the fourth-order hamiltonian does not exceed 3 lattice spacings. It implies that the hamiltonian can be written as a sum over 3×3 plaquettes. Let us choose one family of configurations with density $\rho = \frac{1}{9}$. Now, look at one given configuration (say, No. 1). It is seen that it can be 'glued' from three plaquette configurations (they are marked on Fig. 4, phase $N^o = 1$). But they can be 'glued' together in many different ways, giving lattice configurations of *the same* energy. There is no uniqueness in such a 'gluing' procedure, i.e. resulting lattice configuration is non-unique; the configuration No. $1'$ is one of possible examples. (Situation here is similar to that which happens in the second order for phases **D** and **D**′). As a conclusion, this argument proves presence of *infinite* number of configurations, possessing identical density and energy. An analogous situation happens for configurations 3 and 12.

Phase diagrams in orders 2 and 3 are rigorous (by writing out Hamiltonians as sums of m-potentials). Phase diagram in order 4 is only partially rigorous. For six phases: 0, 4, 5, 7, 10, 11 author has found m-potentials in a manner analogous as in refs. 7,10,17. Unfortunately, it has been achieved not for all regions occupied

by these phases, but only in some open subsets of these regions. Moreover, expressions for m-potentials are lengthy and complicated and don't help too much in clarification of the situation. For these reasons, and because the 'rigorous' regions don't cover the whole phase diagram – expressions for m-potentials have been skipped.

An analysis above concerned the 'truncated' phase diagram, i.e. the phase diagram of the fourth-order effective Hamiltonian (8). Which changes can result as an effect resulting from neglected next-order corrections and temperature?

It turns out that the classical Peierls condition is fulfilled for certain open subsets occupied by phases: 0, 4, 5, 7, 10, 11 (it is an immediate consequence of existence of m-potentials; see ref. 26). It turns out that also quantum Peierls conditions are fulfilled (by calculations analogous as in ref. 25). From these facts, it follows that regions occupied by these phases deform in only small manner upon thermal and quantum perturbations. This assertion concerns regions of phase diagram sufficiently far from phase boundaries obtained for fourth-order Hamiltonian. More precisely, it means that the 'excluded' region, where stability does not hold, possess width of the order $p_5(t, t')/U^4$ ($p_5(t, t')$ is some homogeneous polynom in t, t' variables) around the phase-boundary lines of unperturbed diagram[25].

It seems very like that analogous situation (i.e. stability) takes place also for other non-degenerate phases: 2, 6, 8, 9. Although m-potentials for them hasn't been found, it is very like that the Peierls conditions hold also for these phases. It follows from the restricted phase diagram analysis: It turned out that energies of these configurations are divided by a finite (i.e. independent of N) gap from excitations. For this reason, author conjectures that also these phases are stable.

For regions of width of the order of $p_5(t, t')/U^4$ around phase boundaries, one cannot formulate any statements without going into next orders of perturbation theory. These regions, as well as regions occupied by degenerate phases with numbers: 1,3,12 (all of them form very small subset of the phase diagram), can undergo radical changes upon thermal and quantum perturbations, so they are "terra incognita". Perhaps, the approach due to Kotecký et al.[15,21] could be more effective in analyse of such situations. In this approach, one takes into account the 'thermal' and 'quantum' perturbations in one single step. Such combination of 'thermal' and 'quantum' perturbations could be more effective in the process of degeneracy lifting than taking into account only quantum perturbations, as in the present DFFL-B approach[22–25].

5. SUMMARY AND CONCLUSIONS

The effective Hamiltonian and phase diagram for ground states of the $t - t'$ FKM have been determined up to fourth order of perturbation theory. In the second and third order, phase diagram was constructed by rewritting the Hamiltonian as a sum of m-potentials. The phase diagram in the fourth order has been determined

rigorously for some part of parameter space and by the method of restricted phase diagrams for the remaining part.

The phase diagram is considerably more complicated than for the ordinary FKM, but still it is manageable. Thirteen phases are present (plus their "mirrors"); three of these phases are degenerate.

An interesting feature of the phase diagram is presence of anomally large region occupied by the phase 5, appearing in the fourth order (the region has width proportional to second order in the hopping constants instead of fourth order, as one could expect).

Another aspect of results obtained is possible relation to *stripe formation in strongly correlated electron systems* (I thank the referee for this remark). The question of the relation between charge stripes, correlated electrons and high-temperature superconductivity has been asked many times after discovery of stripes in early nineties. Problem of stripe formation has been investigated mainly in the framework of t–J and Hubbard models, by variety of numerical methods. Unfortunately, these studies gave conflicting results[20]. To explain these contradictory observations, one can guess that both states: possessing stripe order and without such an ordering are very close in energy, so the detection of stripes is a delicate problem. On the other hand, appearance of stripe-like orderings in the Falicov-Kimball model is well established, both rigorously and numerically (results of my paper confirm this tendency; I mean appearance of phases 11 and 12). One can ask the question: Does exist some relation between formation of stripes in FK and Hubbard models? At this moment, I don't know definite answer. There are some heuristic arguments supporting existence of such a relation, but it goes beyond the subject of this paper.

In numerous situations examined so far, it turned out that the FKM is sensitive with respect to changes in the model (unlike to such models as, for instance, the ferromagnetic Ising model, which is rather stable against modifications). Inclusion of such changes as an addition of the correlated hopping, or passing to the non-perturbative values of 'coupling constant' t/U, modifies the phase diagram in strong manner. This is the case also for inclusion of the nearest neighbour hopping. The Falicov-Kimball model exhibits enormous richness in its behaviour.

APPENDIX A: (PSEUDO)SYMMETRIES OF PHASE DIAGRAM OF HAMILTONIANS IN ORDERS 2, 3 AND 4

Let us describe (pseudo)symmetries of the phase diagram, corresponding to effective Hamiltonians. We will proceed order-by-order.

In the second order, the Hamiltonian is symmetric with respect to the change $h \to -h$ and $t' \to -t'$. It is obvious that the phase diagram is symmetric with respect to the change $h \to -h$, if one change also configuration to its mirror image.

In the third order, the Hamiltonian is no longer symmetric. However, their ground states are easily determined, because the Hamiltonian is expressible as a sum of m-potentials, defined on 2×2 plaquettes. It turns out that on the phase diagram, there are present *the same* phases as in the second order. The difference between phase diagrams in the second and third order appears as a change in location of phase boundaries; corresponding lines are shifted by a factor proportional to tt'^2/U^2. This shift is *symmetric* with respect to the change $h \to -h$. In the other words: If some boundary between phases i and j is shifted by ϵ for $h > 0$, then, for $h < 0$, the boundary between mirrors of phases i and j is shifted by $-\epsilon$.

Let us analyse (pseudo)symmetries of the fourth order phase diagram. It turns out that for every phase i appearing for $h > 0$, there exists corresponding mirror $\hat{i}$ for $h < 0$. Phase boundaries between phases i and j and their mirrors $\hat{i}$ and $\hat{j}$ are related by:

$$h_{i/j} = At^2 + A't'^2 + Bt^2t' + Ct^4 + C't^2t'^2 + C''t'^4$$
$$h_{\hat{i}/\hat{j}} = -At^2 - A't'^2 + Bt^2t' - Ct^4 - C't^2t'^2 - C''t'^4$$

which can be seen by taking into account symmetry or antisymmetry of multispin interactions. Let us stress that this situation (i.e. the same structure of phase diagram for $h > 0$ and $h < 0$ is a very peculiar property of the fourth-order Hamiltonian (6), (7), (8). For more general Hamiltonian, we have no such similarity.

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