2D FALICOV–KIMBALL MODEL WITH CORRELATED HOPPING IN THE LARGE U LIMIT*

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Two-dimensional spinless Falicov–Kimball Model (FKM) with a generalized correlated hopping is studied perturbatively in the limit of large on-site Coulomb interaction U. In the half-filled case (*i.e.* $\rho_i + \rho_e = 1$, where ρ_i, ρ_e are densities of ions and electrons, respectively,) an effective Hamiltonian in spin variables is derived up to terms proportional to U^{-3}. Unlike the simplest FKM case, it contains odd parity terms (resulting from the correlated hopping) in addition to even parity ones. The ground-state phase diagram of the effective Hamiltonian is examined in the (a, g, h) parameter space, where a, g are parameters characterizing strength of the correlated hopping and h is a difference of chemical potentials of two sorts of particles present in the system. It appears to be asymmetric with respect to the change $h \to -h$ and a new ordered phases are found for certain values of a and g.

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1. Introduction

The FKM has been originally proposed to describe metal-insulator transition in some rare earth compounds [1]. Later on, the spinless version of the model (that can be viewed as a simplified version of the Hubbard model,

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where spin down (up) electrons are itinerant, whereas spin up (down) electrons are localized), was considered also in a context of mixed valence phenomena [2], crystallization and alloy formation [3], *etc.*

However, it turns out that more adequate description of real systems is attained if a so called *correlated hopping* is taken into account [4–7], *i.e.* when electron hopping amplitudes depend on occupation of a "start" and a "target" lattice sites.

We mainly focus on an influence of correlated hopping on ordering of the localized particles. In our previous paper we examined a simple case, where correlated hopping was determined by a single parameter a [8]. The aim of present work is to investigate a more general three-parameter model. In this model hopping amplitudes may vary independently in the following three cases: when an electron jumps between two occupied sites; when it jumps between two empty sites; when it jumps between one occupied and the other empty site. Therefore, an additional correlated hopping parameter g is introduced.

2. The model

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

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

where

$$H_{0,\Lambda} = U \sum_{x\in\Lambda} w_x n_x - \mu_i \sum_{x\in\Lambda} w_x - \mu_e \sum_{x\in\Lambda} n_x\,, \tag{1}$$

$$V_\Lambda = -\sum_{\langle xy\rangle} \Big[t + a(w_x + w_y) + g w_x w_y\Big] \left(c_x^\dagger c_y + c_y^\dagger c_x\right). \tag{2}$$

Here $c_x^\dagger$ and c_x are creation and annihilation operators of an electron at lattice site $x \in \Lambda$. The corresponding particle number operator is $n_x = c_x^\dagger c_x$ and w_x is a classical variable assuming values 0 and 1; it measures the number of ions at lattice site x. The chemical potentials of ions and electrons are μ_i and μ_e, respectively. The symbol $\langle xy\rangle$ denotes an unordered pair of nearest neighbor sites of the lattice. The parameters a, g appearing in (2) are *correlated hopping constants* (for $a = g = 0$, the model reduces to the ordinary FKM).

3. Perturbation scheme

In this work we examine properties of the model *in the perturbative regime*, *i.e.* in the range of parameters t, a, $g \ll U$, following the method

developed in a series of papers by Datta, Fernandez and Fröhlich [9] (and references therein). Other perturbative schemes have been previously applied to the simplest, *i.e.* without correlated hopping, FKM (and some similar models) [9,10].

In real systems, it has been found that $|a/t| \approx 0.3$ [4,5]. Presumably, the value of $|g/t|$ is even smaller, however, we were not able to find any estimations in the literature. Here we consider the following range of parameters: $-t \le a \le t$, $-t \le g \le t$.

4. Effective Hamiltonian

After some straightforward but lengthy calculations, partially performed with an aid of symbolic computations on a computer, we have obtained the following effective Hamiltonian (describing a low-energy behavior of the system) up to fourth order of the perturbation theory:

$$H_{\rm eff}^{(4)} = \tilde{h} \sum_i S_i^3 + J \sum_{d(i,j)=1} S_i^3 S_j^3 + J' \sum_{d(i,j)=\sqrt{2}} S_i^3 S_j^3 + J'' \sum_{d(i,j)=2} S_i^3 S_j^3$$

$$+ J_{3s} \sum_{\mathcal{S}_{3,ijk}} S_i^3 S_j^3 S_k^3 + J_{3b} \sum_{\mathcal{B}_{3,ijk}} S_i^3 S_j^3 S_k^3 + J_4 \sum_{\mathcal{P}_{4,ijkl}} S_i^3 S_j^3 S_k^3 S_l^3 + J_0 \sum_{\mathcal{P}_{4,ijkl}} \mathbf{1}\,, \quad (3)$$

where $S_x^3 = w_x - \frac{1}{2}$, $\mathcal{B}_{3,ijk}$ "bended" triples; $\mathcal{S}_{3,ijk}$ "straight" triples; $\mathcal{P}_{4,ijkl}$ 2×2 plaquettes on the lattice. The coupling constants in (3) are:

$$\begin{aligned}
\tilde{h} &= h - \tau^3 t_{\rm eff}(10\alpha\gamma + 5\gamma^2 + 20\alpha + 10\gamma)\,,\\
J &= 2\, t_{\rm eff}\tau - 18\, t_{\rm eff}\tau^3\,,\\
J' &= \tau^3 t_{\rm eff}(6 + 8\alpha^2 + 8\alpha\gamma + 2\gamma^2)\,,\\
J'' &= t_{\rm eff}\tau^3(4 + 2\alpha^2 + 2\alpha\gamma + \gamma^2 + 2\gamma)\,,\\
J_{3s} &= t_{\rm eff}\tau^3(4\alpha\gamma + 2\gamma^2 + 8\alpha + 4\gamma)\,,\\
J_{3b} &= t_{\rm eff}\tau^3(8\alpha\gamma + 4\gamma^2 + 16\alpha + 8\gamma)\,,\\
J_4 &= t_{\rm eff}\tau^3(40 + 32\gamma + 8\gamma^2)\,,\\
J_0 &= t_{\rm eff}\tau^3\left(\tfrac{3}{2} - 3\gamma - 2\gamma^2 - 5\alpha\gamma - 5\alpha^2\right),
\end{aligned}$$

where $t_{\rm eff} = t + a$, $\alpha = a/t_{\rm eff}$, $\gamma = g/t_{\rm eff}$, $\tau = t_{\rm eff}/U$, $h = \mu_i - \mu_e$.

Remark 1. The Hamiltonian (3) corresponds to the Ising-like model with (dominating) antiferromagnetic interactions.

Remark 2. It contains one- and three-spin interactions, so the symmetry $h \to -h$ does not longer hold.

5. The phase diagram

We looked for ground states of the Hamiltonian (3) by minimizing energy in some set of "trial" configurations (the method of *restricted phase diagrams*, [11]). We took a set of all *periodic* configurations, having up to 16 sites in an elementary cell. There are 2×23755 such nonequivalent configurations, but it appeared that *all* ground-state configurations have no more than 5 sites per elementary cell. It suggests that configurations with high periods cannot form ground-state phases and presumably our configurations are true minimizers (however, at present we are not able to prove it rigorously).

The phase diagram is displayed in Fig. 1 in a form of slices g =const. for a set of values of g. (More detailed derivation of the effective Hamiltonian and description of the phase diagram we plan to give elsewhere.)

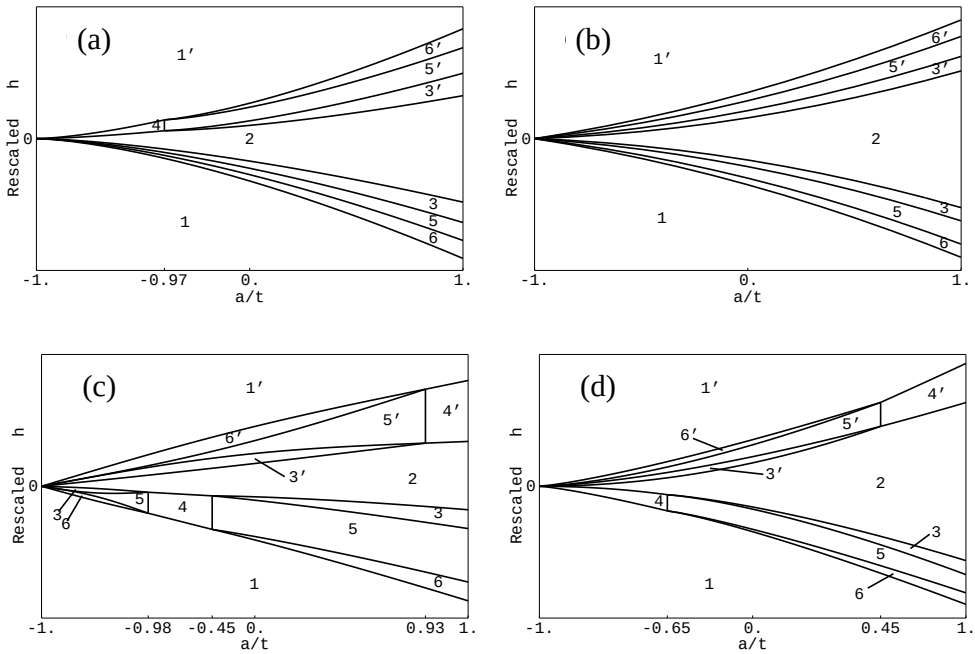

Fig. 1. Schematic phase diagram of the effective Hamiltonian (3) of the correlated hopping FKM. These phase diagrams, together with values of a for boundaries between phases 4/5 or $(4'/5')$ (when present) have been obtained for: (a) $g=-0.8$; (b) $g=-0.6$; (c) $g=0.37$; (d) $g=0.8$. Phases represented by various arrangements of the ions are depicted in Fig. 2.

In the region I, characterized by $-1 \leq g < g_1^*$ ($g_1^* = 1-\sqrt{3} \approx -0.732051$), the phase diagram has a structure displayed in Fig. 1(a), where a small region occupied by the phase $4'$ appears.

In the region II, given by: $g_1^* < g < g_2^*$, where $g_2^* = 1 - \sqrt{7/3} \approx -0.527525$, the ground-state structure is analogous to that of the ordinary FK model for all values of a. (Fig. 1(b)).

In the region III, given by: $g_2^* < g < g_3^*$, where $g_3^* = -3 + \sqrt{11} \approx 0.316625$, the phase diagram structure is similar to the one found by us previously for $g = 0$ [8]. It is characterized by appearance of the new phase 4 and disappearance of some others (3, 5, 6) for certain interval of negative values of a.

In the region IV, given by: $g_3^* < g < g_4^*$, where $g_4^* = 1-\sqrt{1/3} \approx 0.42265$, both new phases 4 and $4'$ are present (Fig. 1(c)) in the diagram.

In the region V, given by: $g_4^* < g < 1$, a simplification of the phase diagram is observed. (Fig. 1(d)).

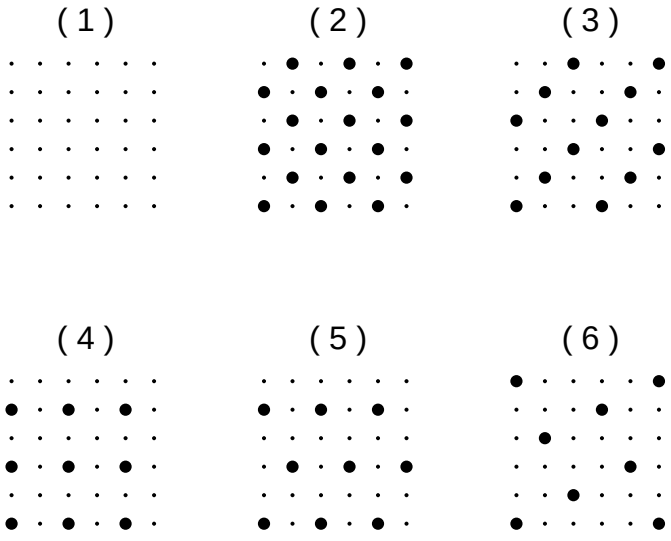

Fig. 2. Configurations of the ions (marked by heavy dots •) corresponding to phases displayed in Fig. 1. Phases labeled by numbers with prime (*e.g.* $1'$, $3'$, $4'$ *etc.*) have mirror configurations with respect to those without prime, *i.e.* lattice sites occupied by the ions are then interchanged with those of unoccupied by the ions.

6. Summary

Our studies indicate an important role of the correlated hopping, as it substantially modifies both the effective Hamiltonian and the phase diagram of the FKM, what can be viewed in Fig. 1. In comparison with our previous studies of the FKM with the single correlated hopping term (proportional to the parameter a), we found that the additional term (measured by the parameter g) not only changes coupling constants of the effective Hamiltonian, but also, within physically admissible values of parameters, it can produce further modification of the phase diagram (*e.g.* new phases can appear on it).

So we conclude that further studies of the model, including its low temperature properties, are highly desirable and hopefully could be useful for description of experimental situations.

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