CORRELATED HOPPING IN THE 1D FALICOV–KIMBALL MODEL*

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Ground state phase diagrams in the canonical ensemble of the one-dimensional Falicov-Kimball Model (FKM) with the correlated hopping are presented for several values of the model parameters. As compare to the conventional FKM, the diagrams exhibit a loss of the particle–hole symmetry.

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As the simplest, still non-trivial model of highly correlated electron systems, the Falicov–Kimball Model (FKM) attracts growing attention among solid state physicists. It can describe variety of the most intriguing cooperative phenomena, as metal-insulator transition, mixed-valence phenomenon *etc.* (see *e.g.* the review [1]).

The model deals with itinerant particles (*e.g.* electrons) that can hope between lattice sites (herein the nearest-neighboring). Some of the sites are occupied by non-movable particles, playing a role of ions or localized electrons; we call them "ions". The only interaction in the system is the on-site, Coulomb-type interaction between the electrons and the ions. The interaction generates long-range ordering of the ions.

The model has been investigated thoroughly in nineties. Numerous approximate results supplemented with some exact and rigorous statements reported up to now provide a good basis for further extensions of the model towards more realistic physical situations. These include the discussed here model with correlated hopping, according to which the electron hopping rate depends on occupations of relevant sites.

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The Hamiltonian of the FKM with correlated hopping reads:

$$H = -t\sum_x \left(c_x^\dagger c_{x+1} + c_{x+1}^\dagger c_x\right)\{1-\alpha[w(x)+w(x+1)-\gamma w(x)w(x+1)]\} + U\sum_x w(x)c_x^\dagger c_x\,, \tag{1}$$

where $w(x)$ denotes the ion occupation number at site x (it takes a value 0 or 1), $c_x^\dagger, c_x$ are the operators that create and annihilate an electron at site x, respectively. Note that with the parametrization given in (1) the hopping amplitudes can take the three following values: $t_{00} = t$ if an electron hops between two empty sites, $t_{01} = t(1-\alpha)$ if it hops between one site occupied by an ion and the other empty (obviously $t_{01} = t_{10}$), and finally $t_{11} = t[1-\alpha(2-\gamma)]$ if it hops between two sites occupied by ions. For $\alpha = 0$ the Hamiltonian (1) reduces to the conventional FKM without correlated hopping.

The meaning of the correlated hopping parameters α and γ depends on a particular physical situation to be modelled. For instance, the α parameter may originate from *bond-charge* repulsion, the mechanism originally discussed in frames of the extended Hubbard model [2,3]. Within the same microscopic picture the parameter γ depends strongly on the effective nuclear charge Z and apparently decreases for larger Z [3].

In general, recognition and understanding the mechanisms leading to the correlated hopping, as well as its consequences are far from being satisfactory. In particular, this concerns the problem of formation of stable phases. The present work turns towards this direction for the simplest, one-dimensional case.

Various approaches known for the ordinary FK model have been adopted to its extended version [4]. Here we used an approximate method of *restricted phase diagrams*, where infinite systems of periodic phases, whose period does not exceed some $r_{\max}$, as well as their mixtures were considered. In this paper we put $r_{\max} = 7$, the value large enough to see main new features of the diagrams. The Gibbs potentials of all these periodic phases were calculated exactly [5], so we were able to get the phase diagrams in the grand-canonical ensemble (in a (μ_e,μ_i) plane) with a high precision. Then we mapped them onto the (ρ_e, ρ_i) plane, thus obtaining canonical phase diagrams. Details of the method and the calculation procedures were published previously (see [6, 7]).

Our results are presented in Fig. 1, where we took the intermediate value of U being equal to $1.6\,t$, $\alpha = 0$, 0.1, 0.2 and $\gamma = 0.0$, 0.5. Fig. 1(a) corresponds to the simplest FKM, with no correlated hopping terms ($t_{00} = t_{01} = t_{11} = t$). In this case the diagram is symmetric with respect to

exchange between sites occupied by the ions and those unoccupied (it has *the particle–hole symmetry*). An extended analysis of that case was given previously in [7], where arrangements of the ions in the periodic phases were also displayed; here we included the diagram only as a reference one.

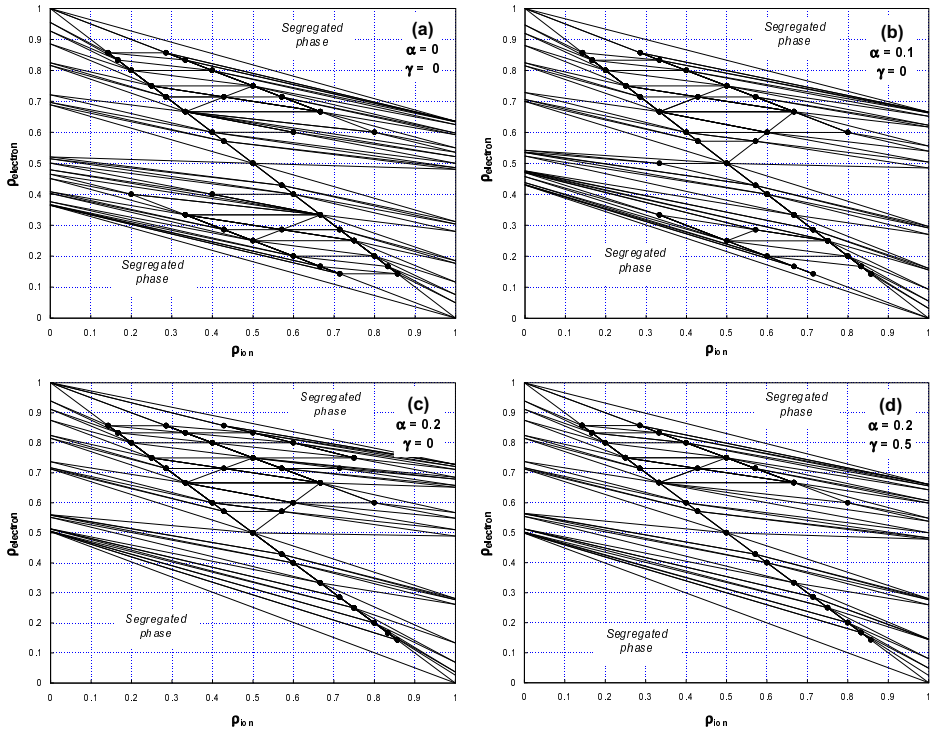

Fig. 1. The restricted canonical phase diagrams for $U = 1.6t$ and the following four sets of correlated hopping parameters: (a) $\alpha = 0$ and $\gamma = 0$; (b) $\alpha = 0.1$ and $\gamma = 0$; (c) $\alpha = 0.2$ and $\gamma = 0$; (d) $\alpha = 0.2$ and $\gamma = 0.5$. The black spots represent periodic phases (whose period is at least 2). The straight line segments join those spots whose corresponding phases touch each other on the phase diagram in the grand-canonical ensemble. The points located on a segment represent the mixtures of the two periodic phases that correspond to the ends of the segment. The black spots located on the lines $\rho_i = 0$ or $\rho_i = 1$ show the minimal and maximal electron densities of the full phases that form mixtures with the same periodic phase.

If one "turns on" the correlated hopping in such a way that $\alpha \neq 0$ and $\gamma = 0$ — see Fig. 1(b), (c), then with an increasing α the diagram becomes more and more asymmetric. For $\alpha = 0.2$ ($t_{00} = t$, $t_{01} = 0.8t$ and $t_{11} = 0.6t$), all periodic phases laying on the left from the $\rho_i + \rho_e = 1$ line disappear and

their place take mixtures of periodic neutral phases with the "empty" one (with free electrons and no ions). Instead the the so-called *three-molecular* periodic phases [7] develop on the right hand side from the $\rho_i + \rho_e = 1$ line.

On the other hand, if we increase the electron hopping amplitude between two occupied sites t_{11} from $0.6t$ to $0.7t$ (what corresponds to $\alpha = 0.2$ and $\gamma = 0.5$ — see Fig. 1(d)), then those *three-molecular* phases are suppressed.

A very brief analysis of the displayed phase diagrams show their considerable sensitivity to a variation of the correlated hopping parameters. In particular, the regions enclosed within the triangles close to the lower-left and upper-right corners of the diagrams, where *the segregated phase* (a mixture of an empty lattice with free electrons and the fully occupied lattice with a number of electrons) is stable, clearly depends on values of the correlated hopping amplitudes (see Fig. 1). The above preliminary results confirm conjectures already published several years ago (*e.g.* [3]), that the correlated hopping plays an important role and should be taken into account if one intends describe properly physical properties of the systems.

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