

DOPING INDUCED TRANSITION FROM AN ANTIFERRO-TYPE ORDER TO PHASE SEPARATION*

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(Received July 10, 2002)

A sequence of transitions from an antiferro-type order to a phase separate state under doping away from half filling is studied within the 1D Falicov–Kimball model. Using the method of restricted phase diagrams the system is analyzed exactly in the thermodynamic limit. Various kinds of ordering, including periodic *n-molecular* phases and their mixtures are found for a set of values of the interaction constant U .

PACS numbers: 05.30.Fk, 71.30.+h

Some *f-electron* compounds exhibit unusual thermodynamic and transport properties, where temperature, external magnetic field, pressure, or doping (chemical pressure) induce a transition from an insulating or semi-metallic, antiferromagnetic (AF) state with the *f(d)-ions* of integral-valence to a nonmagnetic or ferromagnetic mixed-valent metal [1]. Competition between band effects and localization due to correlations is expected to be a main mechanism responsible for the observed anomalies. To understand the underlying physics, various models of highly correlated system are currently a subject of intensive studies, among which the 1D Falicov–Kimball model (FKM) [2] is one of the simplest, still nontrivial one.

The FKM, although formulated over thirty years ago, reentered in the last decade with a number of works reporting both rigorous theorems, exact and approximate numerical results and various applications [3].

It describes two kinds of particles on a periodic lattice: *electrons* and *ions*. The ions occupy some of the lattice sites; they don't move. The electrons can hope between neighboring lattice sites with the amplitude t

* Presented at the International Conference on Strongly Correlated Electron Systems, (SCES 02), Cracow, Poland, July 10–13, 2002.

(being the energy unit throughout this paper) and interact with the ions via on site δ -like potential U . The Hamiltonian reads

$$H = -t \sum_{\langle i,j \rangle} c_i^\dagger c_j + U \sum_i c_i^\dagger c_i w_i, \quad (1)$$

where i, j run over lattice sites, c_i^\dagger (c_i) are the electron creation and annihilation operators respectively, w_i is equal to 1 if site i is occupied by an ion or 0 otherwise. Each ion configuration is identified by a set $[w_i]_r$ of r values of w_i (0 or 1) for i ranging from one to the period r .

One of the characteristic features of the phase diagram, which we would like to focus on in this report, is a presence of two characteristic phases for any value of the on site interaction parameter U [4]:

- AF-type — chessboard phase for $\rho_e = \rho_i = 1/2$ (ρ_e and ρ_i are the electron and ion densities, respectively), where every second site of the 1D crystal is occupied by an ion and the system is an insulator. It can be viewed as an analog of the simplest antiferromagnetic state in the Hubbard model, where spins oriented in one, say up, direction occupy only one of two sublattices.
- SP — segregated phase, being the ground state for sufficiently low value of ρ_e , in which the electrons and the ions avoid each other and reside in separate domains. This phase can be viewed as an analog of the ferromagnetic state in the Hubbard model, where spins up (here representing by the ions) clump together, forming a ferromagnetic domain.

Using the method of *restricted phase diagrams* [5,6], we have taken into account all admissible periodic arrangements of the ions $\{w\}$, for which the period r does not exceed 16. For each configuration w and a set of interaction constant values U , the total energy as a function of chemical potentials of the electrons (μ_e) and ions (μ_i) has been determined. The ground state configurations obtained from the minimization procedure and mapped onto the plane (μ_e, μ_i) constituted the zero temperature *restricted phase diagram* of the system in the *grand canonical ensemble*. Then it was translated to the complementary restricted phase diagram in the *canonical ensemble* in the (ρ_e, ρ_i) plane.

The calculations have been performed for twenty values of U : 0.1, 0.2, 0.3, 0.4, 0.6, 0.8, 1.0, 1.4, 1.6, 1.8, 2.0, 2.6, 3.0, 3.4, 3.8, 4, 6, 8, 12, 16. The number of ground state configurations that appear on the phase diagram depends on U , ranging from 21 for $U = 16$ up to 169 for $U = 0.1$. Hereafter the discussion is restricted to phases defined by the constraint $\rho_e = \rho_i = \rho$. This assumption corresponds to $S_z = 0$ limit in the Hubbard model.

Results of analysis of the canonical phase diagrams for the values of U are shown in Fig. 1. For a large interaction constant U , apart from SP, only mixtures of the empty ($\rho_i = 0$) and the most homogeneous periodic phases are stable. The region where they appear is close to the half-filling. Its width falls to zero as U tends to infinity [4] and the number of different periodic configurations that participate in the mixtures decreases. In the limit of U infinite only the chessboard phase and other the most homogeneous phases survive.

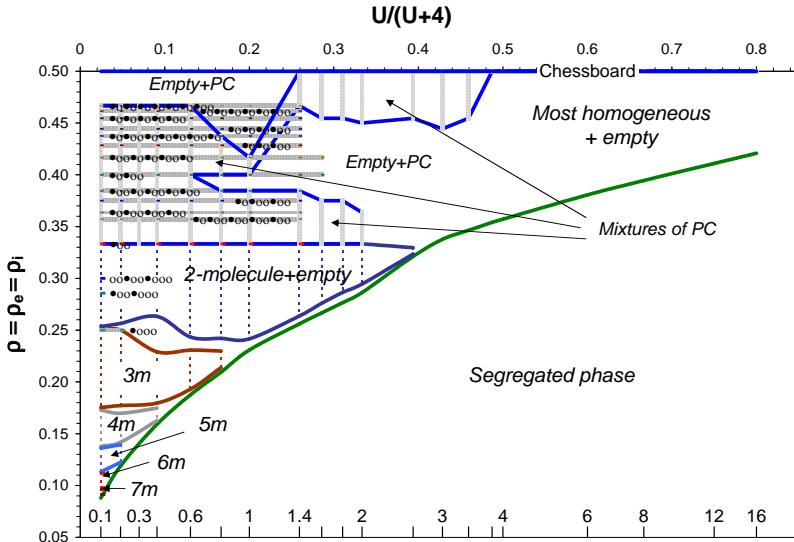


Fig. 1. Phase diagram of the 1D FKM along the $\rho_e = \rho_i$ line for a set of U values marked on the lower axis.

The diagram becomes much more complicated for intermediate and small values of U , where additional families of ordered phases appear. These are periodic configurations (PC) other than the simplest AF-type, their two and three component mixtures and mixtures of PC with the empty phase.

For $U = 2.6$ a new type of structures becomes visible: the most homogeneous *hole two-molecule* configurations [7]. They are characterized by a fixed to two number of neighboring empty sites. Pairs of ion holes are homogeneously distributed in unit cells. In addition, the number of electrons is equal to the number of *hole two-molecules* in these phases. As it can be seen in the Figure 1, there is a relatively large region of coexistence of the *2-molecules* with the empty phase. As U decreases, *3-molecule* mixtures with the empty phase develop for lower densities, then *4-molecule* and so on.

The diagram for intermediate U values, between 0.6 and 3.0, is especially interesting. For instance, for $U = 1.0$ and below the chessboard phase ($\rho = 1/2$) mixtures of periodic phases with the empty phase are present in the following tree regions of ρ : (0.23–0.33), (0.385–0.4) and (0.417–0.5), separated by two areas of mixtures of periodic configurations.

In summary, we studied the one-dimensional FK model in the thermodynamic limit by the method of restricted phase diagrams and showed in detail how the chessboard phase evolves to the segregated phase as a function of doping. It appeared that the ground state changes in a complex way, especially for intermediate and small values of U , where competition between AF-type and SP phase becomes more expressive [8].

Support from the Polish State Committee for Scientific Research (KBN) under Grant no. 2P03B13119 is gratefully acknowledged.

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